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Hybrid parallel programming & advanced topics

Simon Scheidegger
simon.scheidegger@unil.ch
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Including adapted teaching material from books, lectures and presentations by
B. Barney, B. Cumming, W. Gropp, G. Hager, M. Martinasso, R. Rabenseifner, O. Schenk, G. Wellein

Today’s Roadmap:

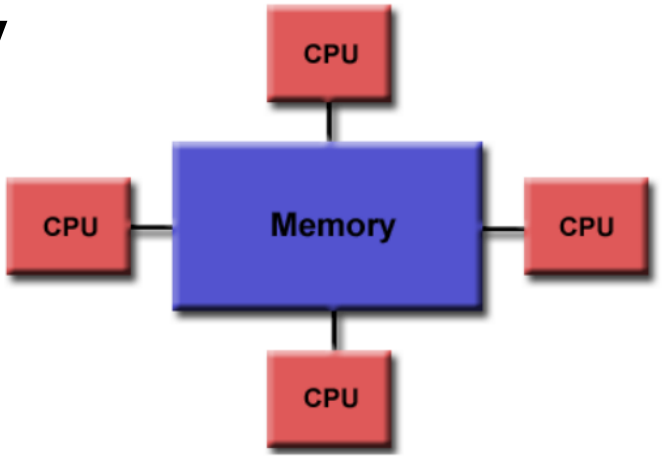
1. Hybrid parallelism.
2. Hybrid parallel Dynamic Programming.
3. Libraries & Advanced topics.

Reminder: Shared memory systems

- Process can access same GLOBAL memory

- Uniform Memory Access (UMA) model

- Access time to memory is uniform.
- Local cache, all other peripherals are shared.

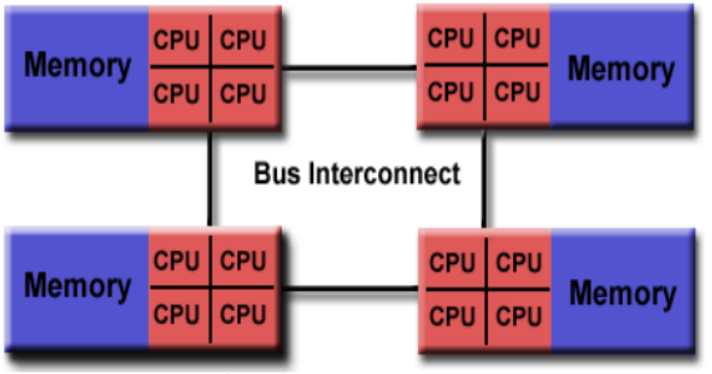


Shared Memory (UMA)

- Non-Uniform Memory Access (NUMA) model

- Memory is physically distributed among processors.
- Global virtual address spaces accessible from all processors.
- Access time to local and remote data is different.

→ **OpenMP**, but other solutions available (e.g. Intel's TBB).

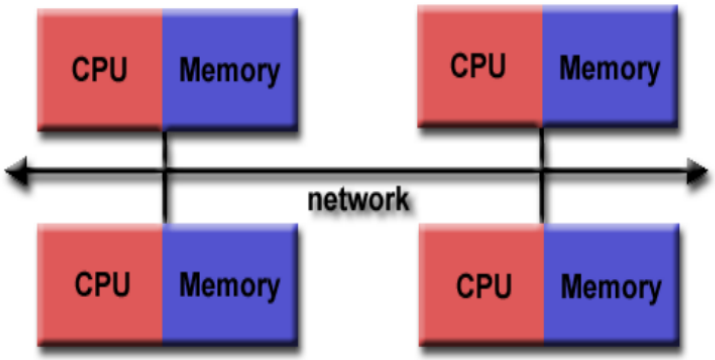


Shared Memory (NUMA)

Reminder: Distributed-memory systems

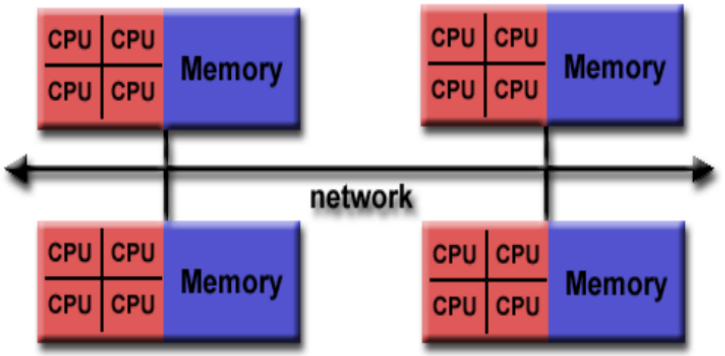
- We need to use explicit message passing,
  i.e., communication between processes:
  → Most tedious and complicated but also
  the most flexible parallelization method.

- Message passing is required if
  a parallel computer is of **distributed-memory**
  type, i.e., if there is no way for one processor
  to directly access the address space of another.



- However, it can also be regarded
  as a programming model and used
  on shared-memory or **hybrid systems** as well.

→ **Message Passing Interface (MPI)**.

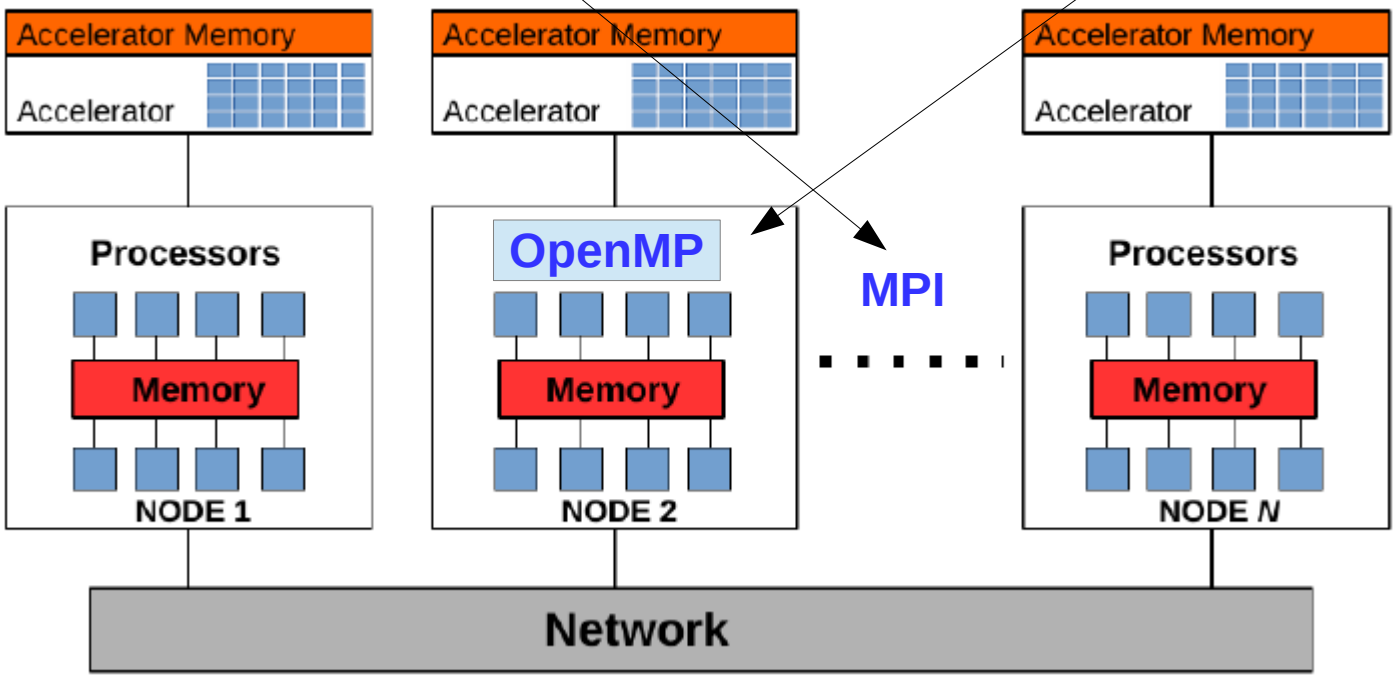


Today's HPC systems

- Efficient programming of clusters of **shared memory nodes**

- Hierarchical system layout

- Hybrid programming seems natural:
  - → **MPI among the nodes.**
  - → **Shared memory programming inside of each node – OpenMP.**



Hybrid parallelism with MPI and OpenMP

When Does Hybridization Make Sense?

- When one wants to scale a shared memory OpenMP application for use on **multiple SMP nodes** in a cluster.

- When one wants to reduce an MPI application's sensitivity to becoming communication bound.

- **When one is designing a parallel program (nowadays) from the very beginning.**

- for 8/16/32/64/...ranks per multi-core node, this can have scaling problems with many nodes/MPI ranks.

Hybridization Using MPI and OpenMP

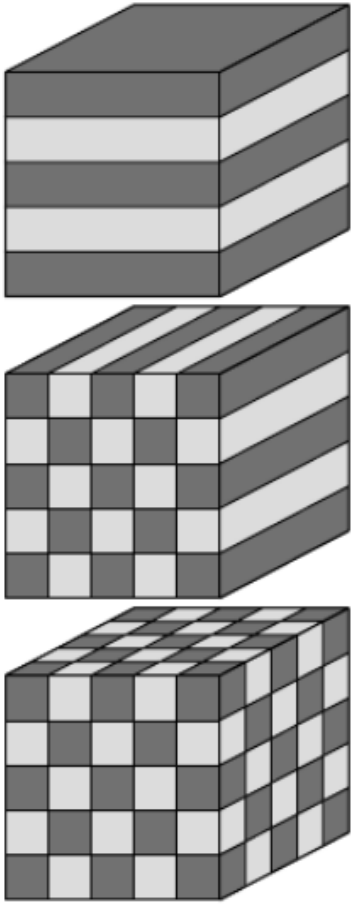
- facilitates cooperative shared memory (OpenMP) programming across clustered SMP nodes.

- MPI facilitates **communication** among SMP nodes.

- OpenMP manages the **workload** on each SMP node.

- **MPI and OpenMP are used in tandem** to manage the overall concurrency of the application.

Domain decomposition & communication

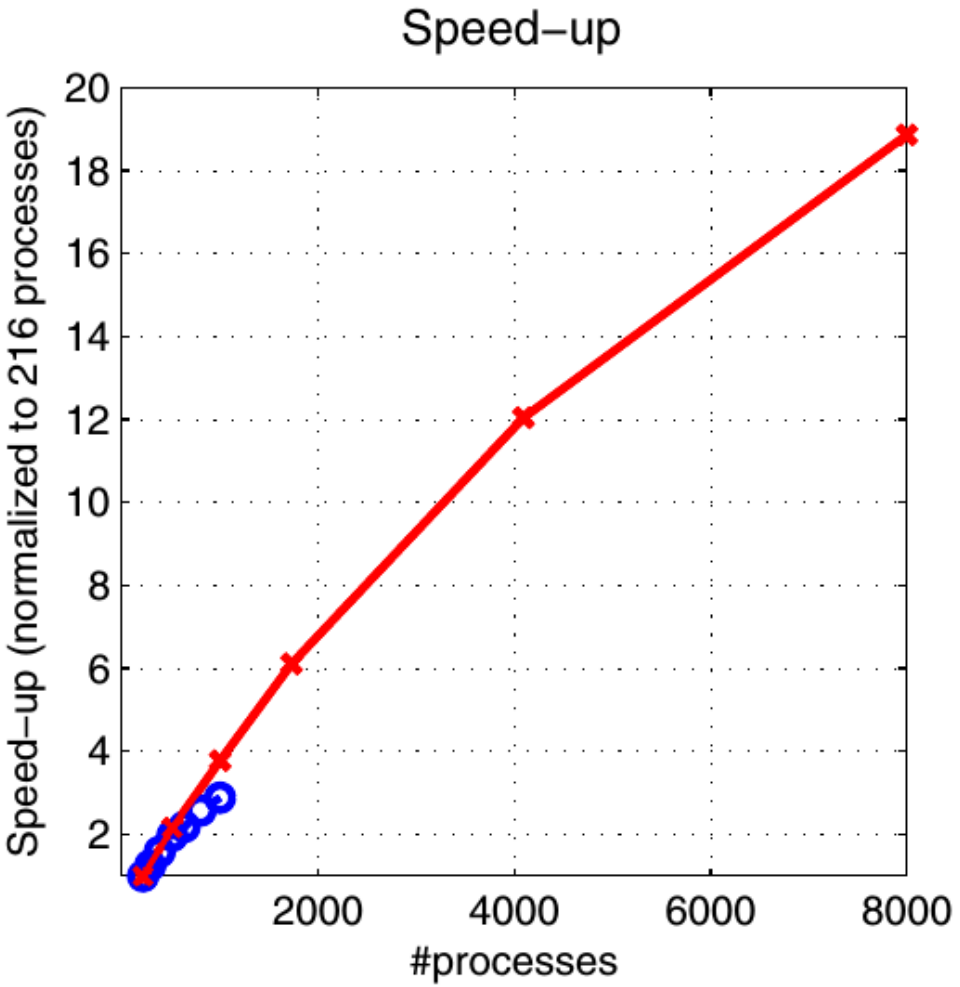


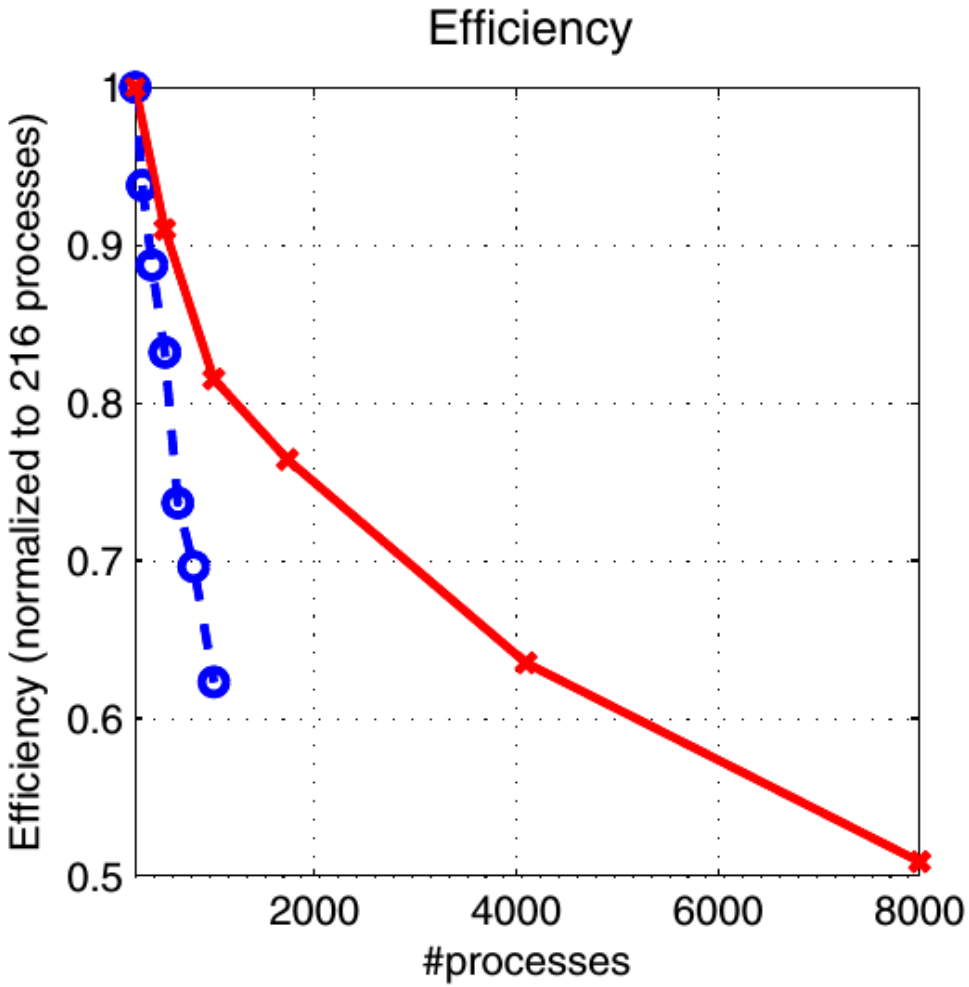
From Hager & Wellein (2011)

Example: Scaling “MPI” vs. “Hybrid”

See, e.g., Käppeli et al. (2011) http://iopscience.iop.org/article/10.1088/0067-0049/195/2/20/pdf

Hybrid parallelization for cubic domain decomposition:
→ Reduces the amount of memory consumption.
→ Reduces the amount of communication required.





Memory consumption & mapping

- Memory consumption MPI & OpenMP with n threads per MPI process:
  → Duplicated data may be reduced by factor *n*.

- How many threads per MPI process?
  SMP node = with *m* sockets (NUMA domains) and *n* cores/socket

- How many threads (i.e., cores) per MPI process?
  → Too few threads, too much memory consumption

- Optimum:
  → somewhere between 1 and m x n threads per MPI process.

- Typical optima:
  → 1 MPI process per whole SMP node.
  → 1 MPI process per socket.
  → 2 MPI processes per socket.

Mapping (1)

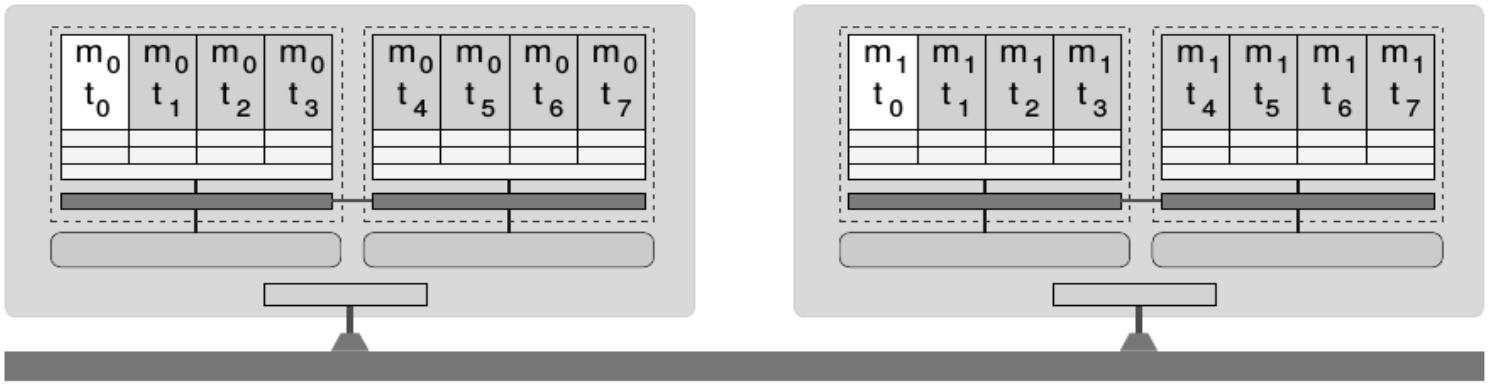


Figure 11.3: Mapping a single MPI process with eight threads to each node.

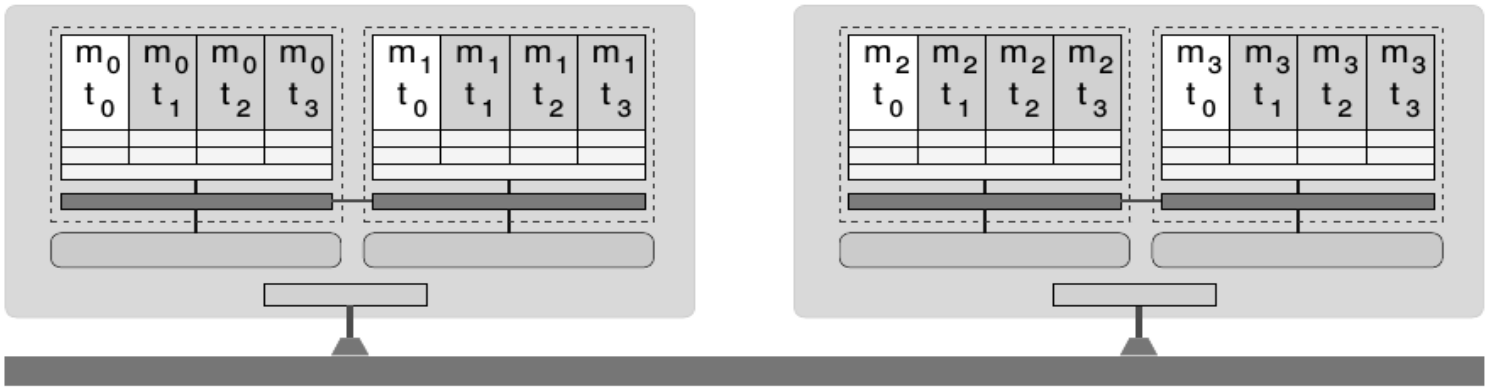


Figure 11.4: Mapping a single MPI process with four threads to each socket (L3 group or locality domain).

From Hager & Wellein (2011)

Mapping (2)

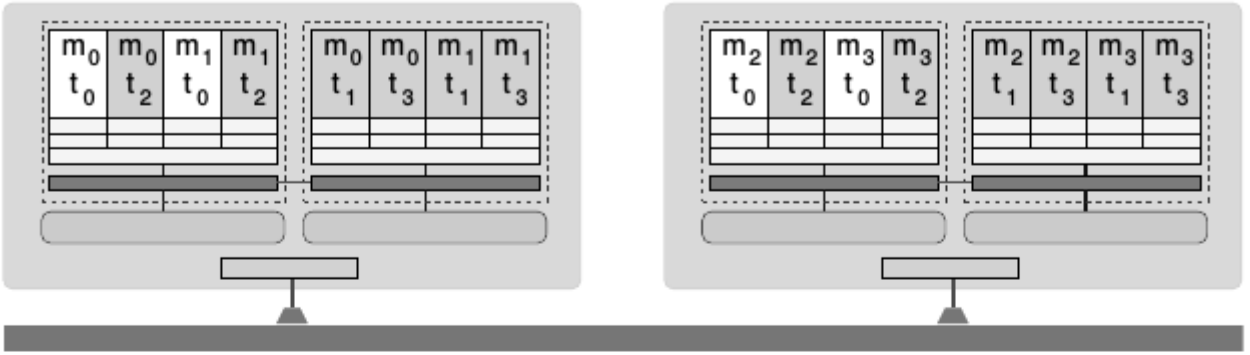


Figure 11.5: Mapping two MPI processes to each node and implementing a round-robin thread distribution.

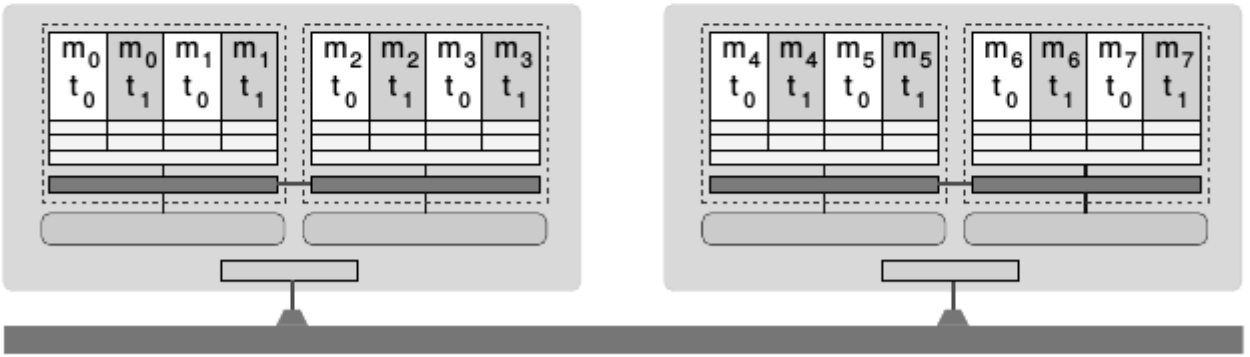


Figure 11.6: Mapping two MPI processes with two threads each to a single socket.

From Hager & Wellein (2011)

Opportunities

Algorithmic opportunities due to larger physical domains inside of each MPI process:

→ If MPI domain decomposition is based on physical zones:
Nested Parallelism Outer loop with MPI / inner loop with OpenMP.

→ Load-Balancing: Using OpenMP dynamic and guided work sharing

→ Memory consumption: Significantly reduction of replicated data on MPI level.

→ Reduced MPI scaling problems: Significantly reduced number of MPI processes

→ Opportunities, if MPI speed-up is limited due to algorithmic problem

→ Significantly reduced number of MPI processes.

A common way to implement hybrid paralleism

Fortran

```
include 'mpif.h'
program hybsimp


call MPI_Init(ierr)
call MPI_Comm_rank (...,irank,ierr)
call MPI_Comm_size (...,isize,ierr)
! Setup shared mem, comp. & Comm

!$OMP parallel do
   do i=1,n
     <work>
   enddo
!  compute & communicate

call MPI_Finalize(ierr)
end
```

C/C++

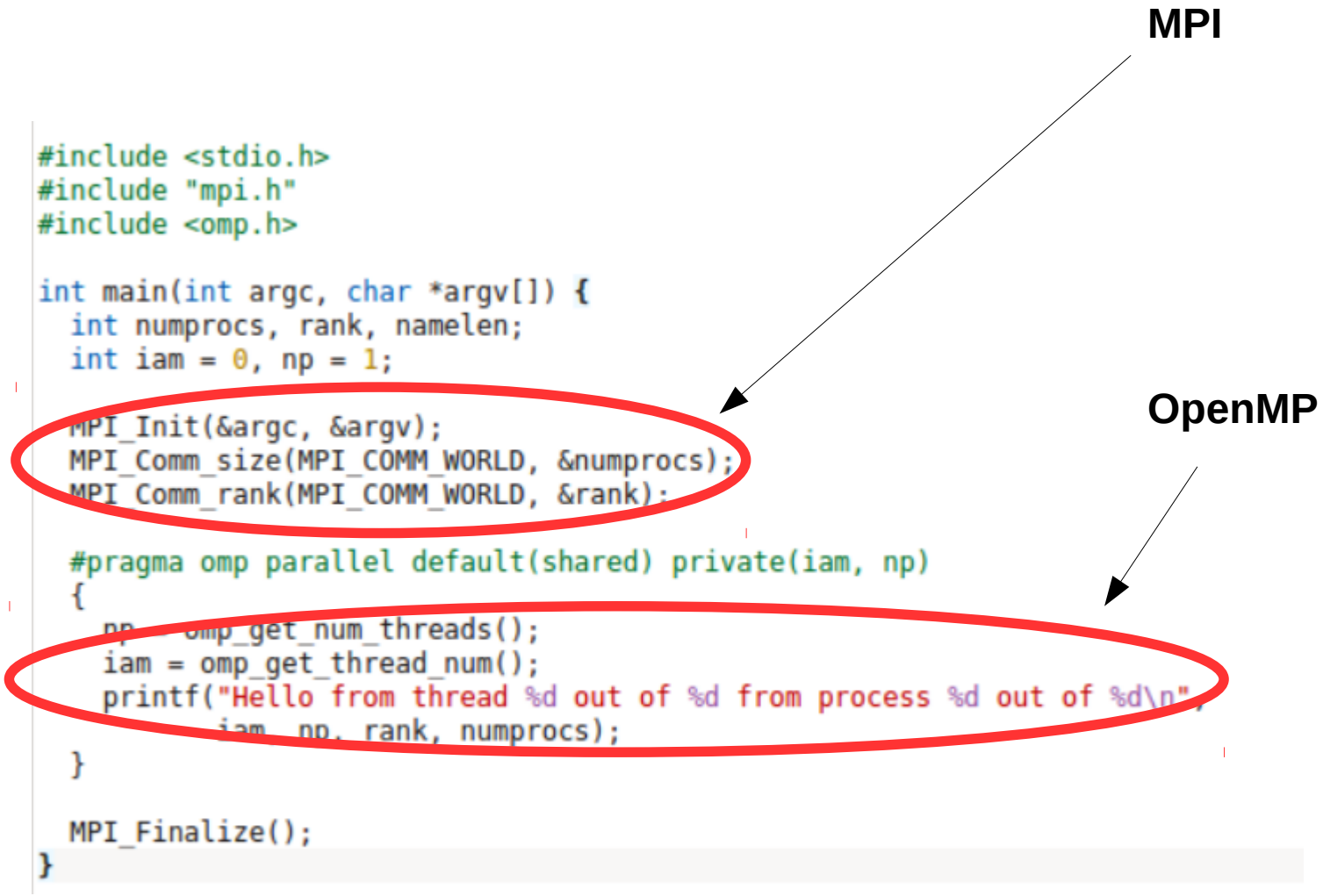
```
#include <mpi.h>
int main(int argc, char **argv){
 int rank, size, ierr, i;

ierr= MPI_Init(&argc,&argv[]);
ierr= MPI_Comm_rank (...,&rank);
ierr= MPI_Comm_size (...,&size);
//Setup shared mem, compute & Comm

#pragma omp parallel for
   for(i=0; i<n; i++){
     <work>
   }
// compute & communicate

ierr= MPI_Finalize();
```

Example




```c
#include <stdio.h>
#include "mpi.h"
#include <omp.h>

int main(int argc, char *argv[]) {
  int numprocs, rank, namelen;
  int iam = 0, np = 1;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  #pragma omp parallel default(shared) private(iam, np)
  {
    np = omp_get_num_threads();
    iam = omp_get_thread_num();
    printf("Hello from thread %d out of %d from process %d out of %d\n",
           iam, np, rank, numprocs);
  }

  MPI_Finalize();
}
```

Example:”hello world hybrid”

1. go to YaleParallel2018/day4/code/hybrid:

> cd YaleParallel2018/day4/code/hybrid

2. Have a look at the code

> vi 1a.hello_world_hybrid.cpp

3. compile by typing:

> source setupenv.sh (load correct MPI library)
> make

```
mpicxx -fopenmp 1a.hello_world_hybrid.cpp -o 1a.hello_world_hybrid.exec
```

4. Experiment with different numbers of threads/MPI Processes

> export OMP_NUM_THREADS=4
> mpirun -np 2 ./1a.hello_world_hybrid.exec

Slurm & Hybrid Jobs on GRACE

```
#!/bin/bash
#SBATCH --job-name=hybrid
#SBATCH --output=hydrid_job.txt
#SBATCH --ntasks=8
#SBATCH --cpus-per-task=5
#SBATCH --nodes=2
#SBATCH --time=10:00
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
mpirun hello_hybrid.mpi
```

→ **8 MPI** processes (***ntasks***), distributed on 2 ***nodes***.
→ 5 threads per MPI process (*cpus-per-task*)
→ 8 x 5 CPUs = 40 CPUs

Example: Slurm on GRACE

1. go to YaleParallel2018/day4/code/hybrid:

> cd YaleParallel2018/day4/code/hybrid

2. Have a look at the code

> vi submit_hybrid_yale.sh

3. compile by typing:

> make

4. Experiment with different numbers of nodes/threads/MPI Processes and look at the output.

> sbatch submit_hybrid_yale.sh

Putting things together: Hybrid parallel DP

recall – the model

$$V_{new}(k,\Theta) = \max_{c} \left(u(c) + \beta \mathbb{E}\{V_{old}(k_{next},\Theta_{next})\}\right)$$

$$\text{s.t.} \quad k_{next} = f(k,\Theta_{next}) - c$$

$$\Theta_{next} = g(\Theta)$$

States of the model:

- k : today's capital stock → **There are many independent k's**
- Θ: today's productivity state → **The Θ's are independent**

Choices of the model:

- k_{next}

→ k, k_{next}, Θ and Θ_{next} are limited to a finite number of values

solver.cpp – the critical loops

```
for (int itheta=0; itheta<ntheta; itheta++) {

    /*
     Given the theta state, we now determine the new values and optimal policies corresponding to each
     capital state.
     */

    for (int ik=0; ik<nk; ik++) {

        // Compute the consumption quantities implied by each policy choice
        c=f(kgrid(ik), thetagrid(itheta))-kgrid;

        // Compute the list of values implied implied by each policy choice
        temp=util(c) + beta*ValOld*p(thetagrid(itheta));

        /* Take the max of temp and store its location.
         The max is the new value corresponding to (ik, itheta).
         The location corresponds to the index of the optimal policy choice in kgrid.
         */
        ValNew(ik, itheta)=temp.maxCoeff(&maxIndex);

        Policy(ik, itheta)=kgrid(maxIndex);

    }
}
```

2). *split MPI communicator

1). distribute k's via OpenMP & MPI

loops to worry about conceptually!

Recall:MPI communicators and ranks

- Every process has an MPI rank and belongs to an MPI communicator.

- An MPI rank is an identification number.

- An MPI communicator is a set of MPI rank.

- Ranks are numbered locally to communicator.

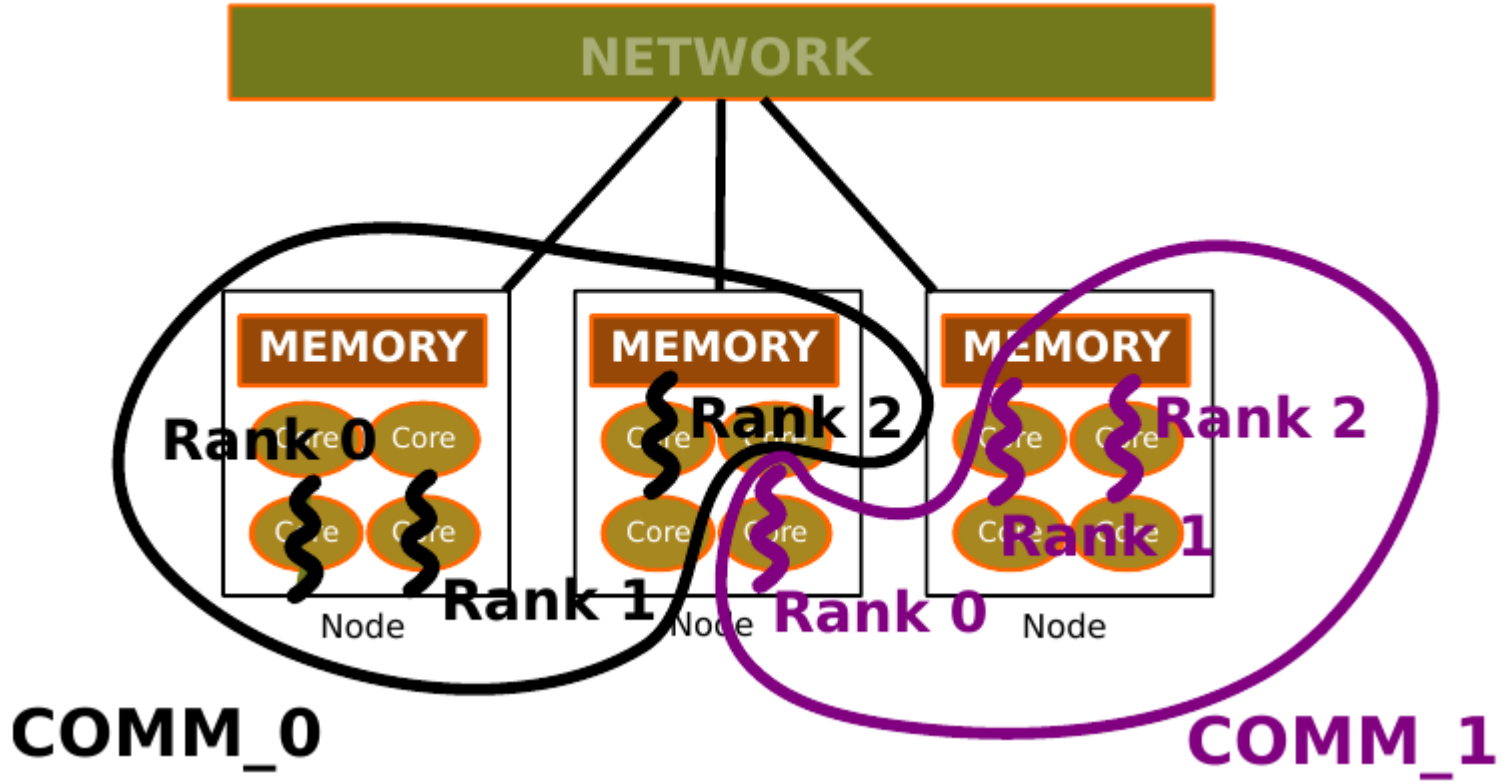
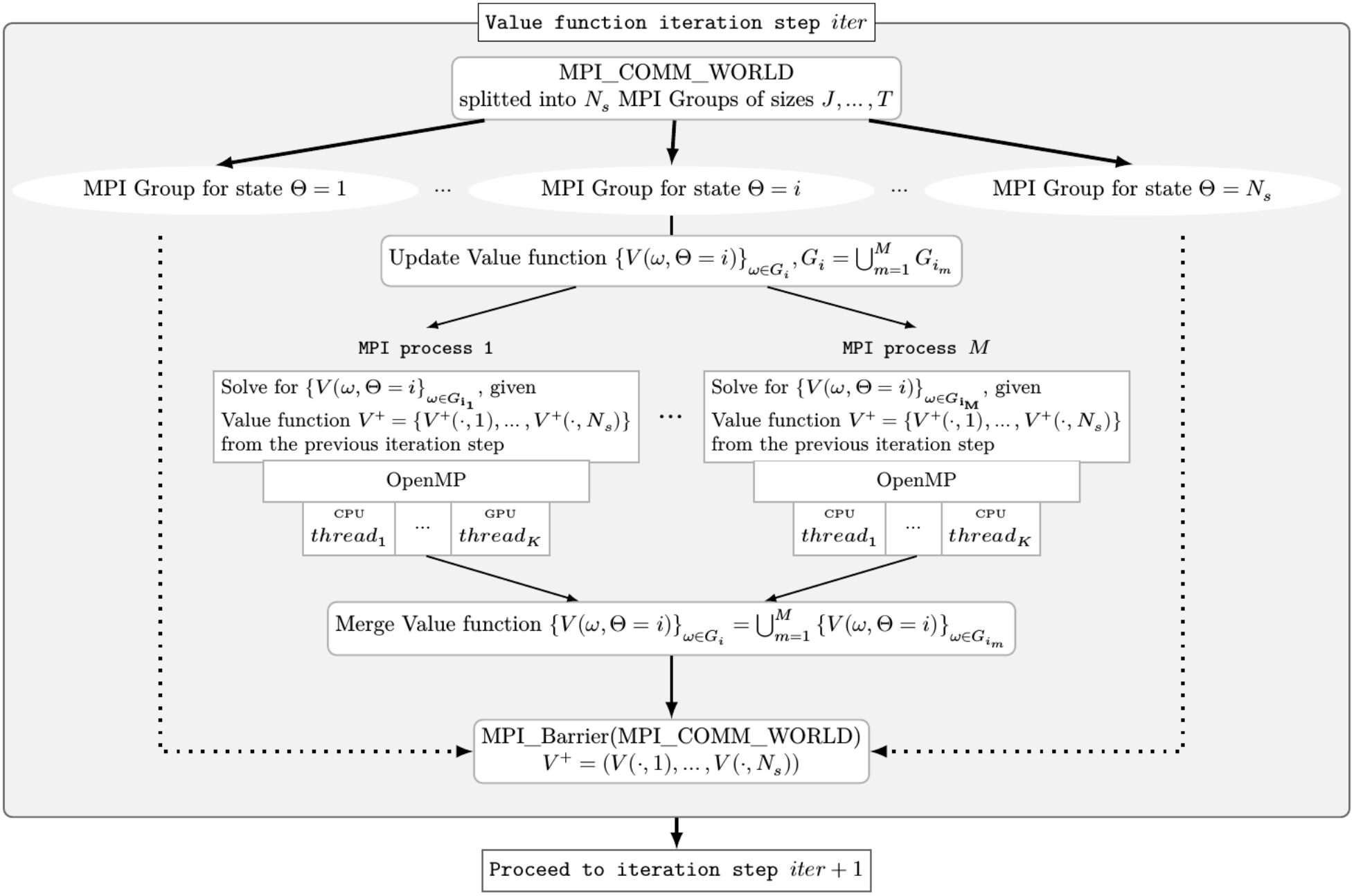
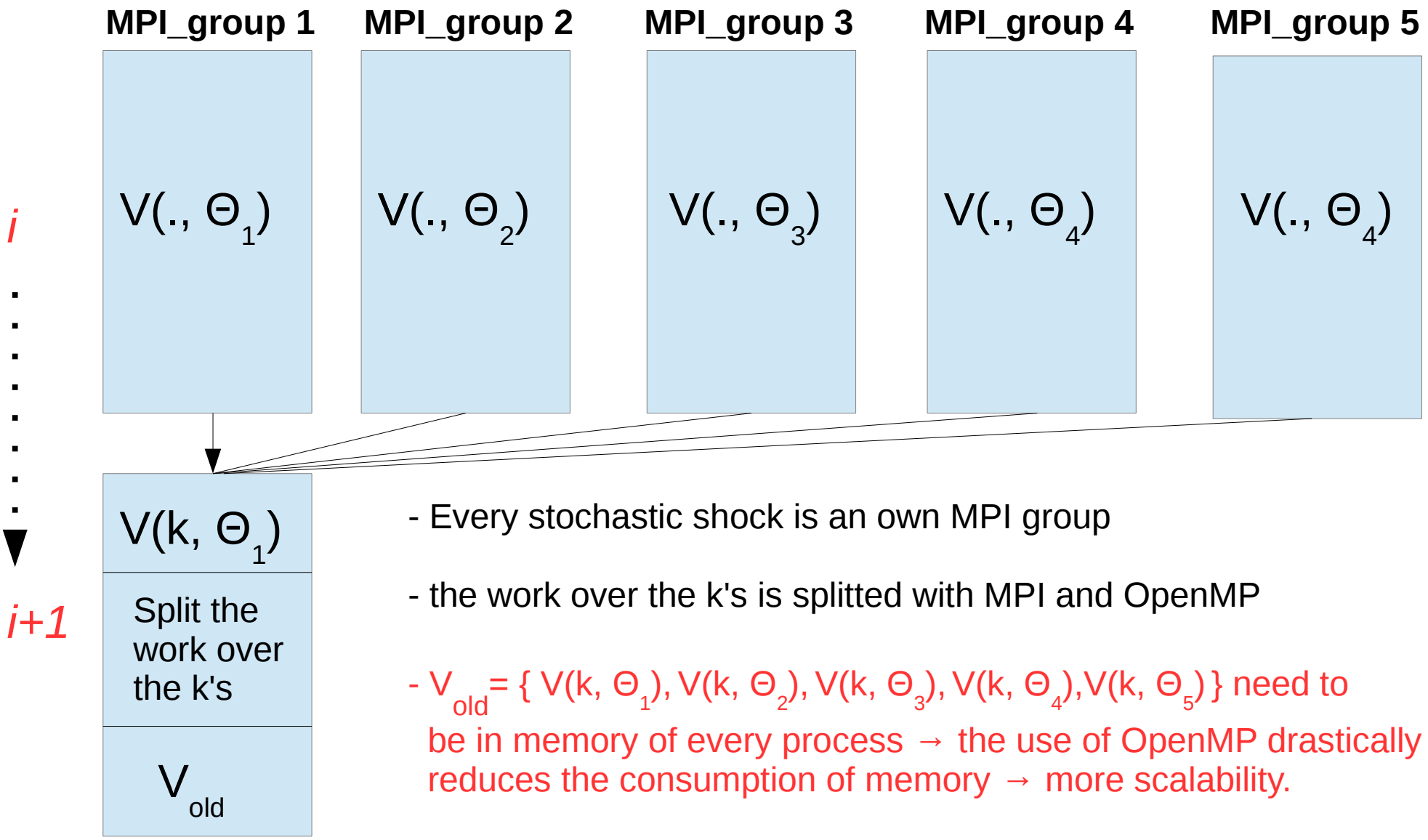


Fig. from M. Martinasso

The parallelization scheme



The parallelization scheme



- Every stochastic shock is an own MPI group

- the work over the k's is splitted with MPI and OpenMP

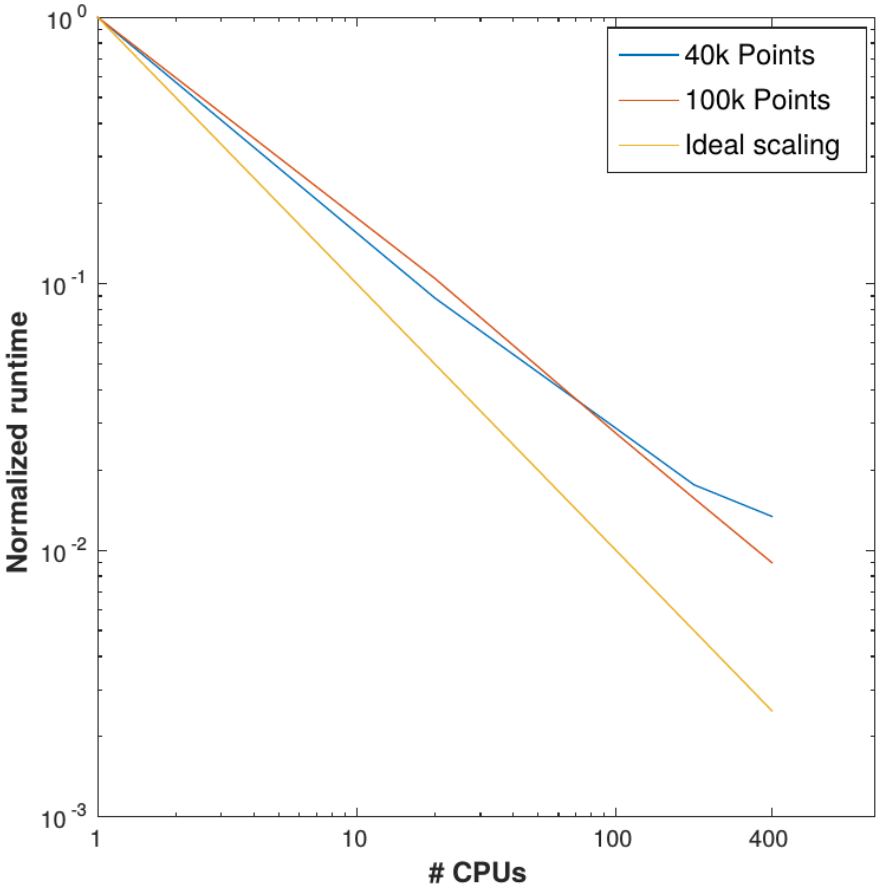
- $V_{old} = \{ V(k, \Theta_1), V(k, \Theta_2), V(k, \Theta_3), V(k, \Theta_4), V(k, \Theta_5) \}$ need to be in memory of every process → the use of OpenMP drastically reduces the consumption of memory → more scalability.

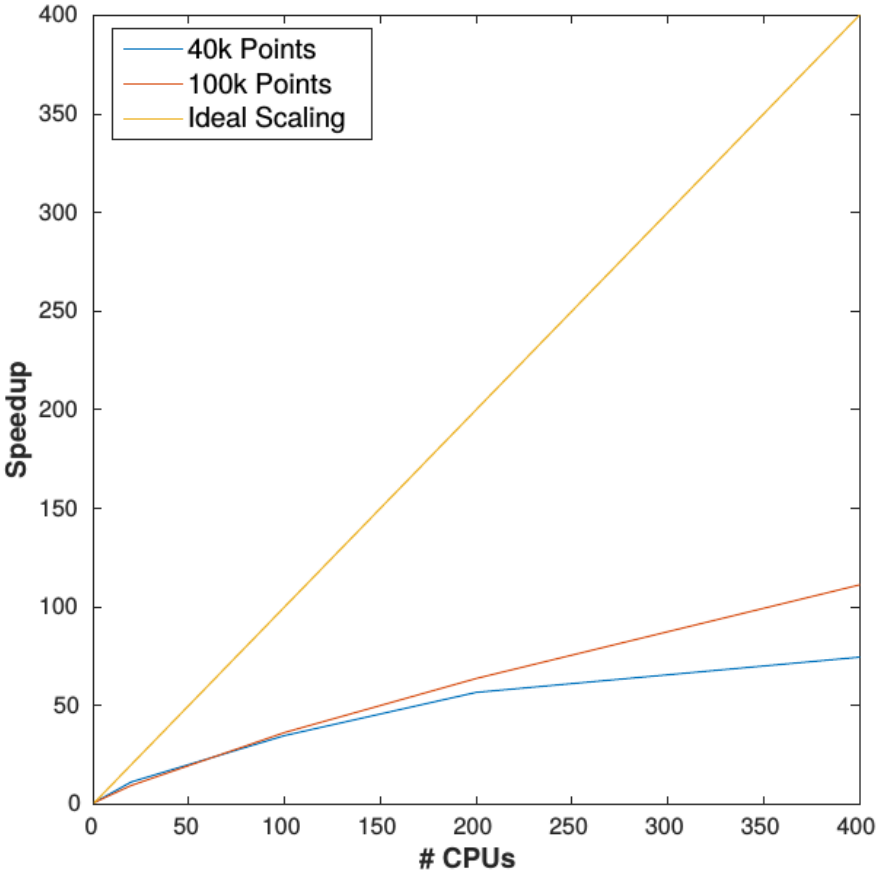
Let's look at the code together!

1) OMP & MPI:
YaleParallel2018/day4/code/DynamicProgramming/DP_hybrid

2) MPI groups:
YaleParallel2018/day4/code/DynamicProgramming/DP_MultComms

Performance: 40 & 100k points





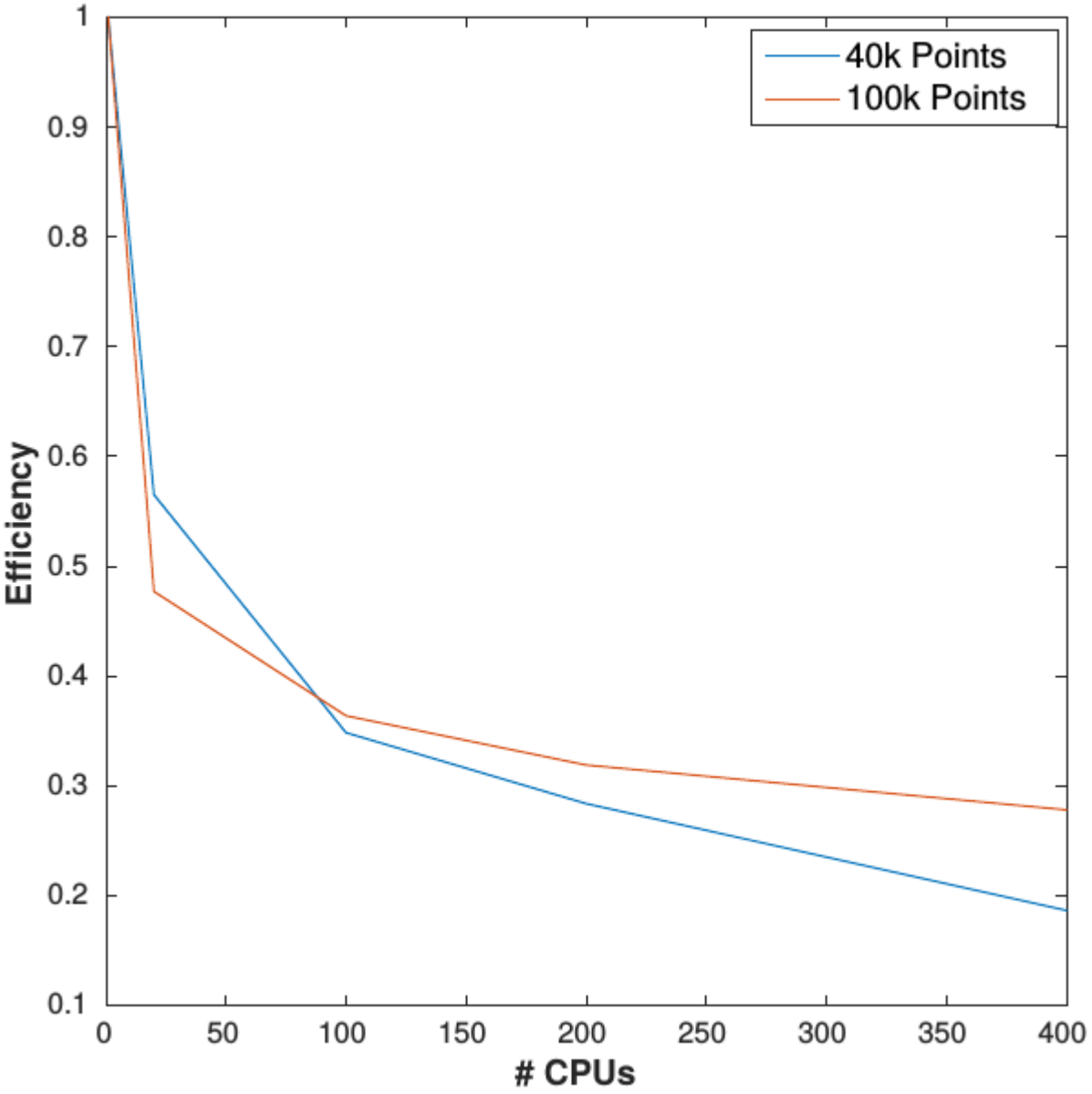
Scalability for this problem size is limited.

→ Overhead quickly becomes dominant: the runtime is ~2 sec for 400 CPUs with 40k points.

→ **Appropriate baseline is probably rather 1 single node**

Efficiency: 40 & 100k points

Model way more than 99% parallel!
→ recall Amdahl's law



Libraries & Advanced topics

1. Libraries

2. Emerging hardware

3. Trending topics

Libraries*

*The other commandments got lost in translation

What is a software library?

- **A set of related functions to accomplish tasks required by more than one application**.

- **Written and used by different people.**

- Relies on an Application Programming Interface (API).

- Typically versioned, documented, distributed, licensed.

Libraries for Scientific Computing: Pros

- **Don’t reinvent the wheel.**

- **Don’t reimplement the wheel.**

- **Use the wheel!**

- Leverage the work of experts.

- **Focus on your part of the “stack” to do science**.

- Experiment quickly.

- **Avoid “lock in”** with respect to data structures and algorithms (maybe a wheel wasn’t the right choice).

- Open source or community projects allow consolidation of efforts from many people.

- **Continuity** on time scales longer than projects/PhDs/grants/careers.

- Collaborative efforts good for science.

Libraries for Scientific Computing: Cons

- Learning curves.

- Versioning, changing APIs.

- Bugs that someone else must fix.

- Syntax, design choices.

- Lack of documentation (or local experts).

- Oversold software.

- The scientific risks of using algorithms (or hardware) that you don’t understand.

Where libraries show up

There are many libraries for scientific computing. Some are specialized to **certain application** areas, others are **quite general**.

- Linear Algebra Libraries
- Sparse Linear Algebra
- Iterative Solvers
- Eigensolvers
- GPU-enabled Linear Algebra Libraries

Examples for general libs.

- SNOPT (optimizer)
- IPOPT (optmizer)

Examples for Specialized libs.

Dense Linear Algebra

- Dense linear algebra, that is – linear algebra on matrices that are stored as two-dimensional arrays has been standardized for a considerable time.

- You almost certainly use these operations already.

- You likely leverage (perhaps indirectly) libraries to do so.

→ Typical Operations include elementary **element-wise operations on matrices and vectors** : A + B,etc.

→ Norms, inner products, matrix-matrix multiplies, matrix-vector multiplies : $||x||_2, \langle x, y \rangle, AB, Ax,$

→ Cholesky factorization: $A = LL^T, L$ lower triangular

→ QR decomposition: $A = QR, Q^H Q = I,\ R$ upper triangular

→ LU factorization: $A = P^T LU,\ P$ permutation, L lower triangle, R upper triangle

→ Triangular solves $y = L^{-1}x$

→ Eigenvalue decomposition: $Ax = \lambda x \iff A = Q\Lambda Q^T,\ Q^H Q = I$

→ Singular value decomposition: $A = U\Sigma V^H,\ U^H H = I,\ V^H V = I$

BLAS

- The basic operations are defined by the three levels of **Basic Linear Algebra Subprograms (BLAS)**:

→ **Level 1** defines **vector operations** that are characterized by a single loop.

→ **Level 2** defines **matrix vector** operations, both explicit such as the matrix-vector product, and implicit such as the solution of triangular systems.

→ **Level 3** defines **matrix-matrix operations**, most notably the matrix-matrix product.

- The name ‘BLAS’ suggests a **certain amount of generality**, but the original authors were clear that these sub-programs only covered dense linear algebra.

- Attempts to standardize sparse operations have never met with equal success.

BLAS & Lapack

- Fundamental numerical libraries.

- Many implementations, optimized for different architectures.

- BLAS

→ vector operations (BLAS-1)
→ matrix-vector operations (BLAS-2)
→ matrix-matrix operations (BLAS-3)

LAPACK

→ Matrix factorization and linear system solution
→ Least squares

SCALAPACK

→ distributed memory LAPACK

- **Available implementations** on compute clusters often include the following:

→ Intel's math kernel library (MKL) includes BLAS and LAPACK,
Cray's libsci : heavily optimized BLAS, LAPACK, SCALAPACK e.g. within the Cray, PGI, and GNU environments.

Example for GPUs: MAGMA

http://icl.cs.utk.edu/magma/

Sparse Linear Algebra

For a tutorial see http://www.users.csbsju.edu/~mheroux/ISC2016HerouxTutorial.pdf

- Use cases: **sparse PDEs, big sparse data**.

- Fundamentally very different from dense linear algebra; operations are difficult to vectorize.

- Typically limited by data movement (memory bandwidth), not floating-point performance.

- Any operator which can be applied (hence potentially inverted) in linear time must be sparse, and most sparse linear algebra libraries are aimed at large systems.

- Efficient for repeated solves suboptimal scaling and entry-dependent factorization time and storage.

- Challenging to parallelize.

- For large-enough systems, eventually beaten by optimally-scaling methods (iterative and/or multilevel algorithms).

Example: http://www.pardiso-project.org/

Download the package
(licence & binary) from there.

You want e.g.
libpardiso600-GNU720-X86-64.so

Add the binary here:
YaleParallel2018/day4/code_day4/pardiso_example/lib

Copy the licence key to a
file named pardiso.lic

Make the licence visible by
a) adding it to your .bashrc
e.g. export PARDISO_LIC_PATH="~/licences/pardiso.lic"

b) putting pardiso.lic to your home directory (cp pardiso.lic ~)

What hardware do you have?

Binaries / Libraries

Current Available Libraries

Version 6.0 (Architecture x86-64, 64-bit)

Compiler	Operating System	PARDISO Libraries
gcc/gfortran 7.2.0	Linux	libpardiso600-GNU720-X86-64.so
gcc/gfortran 8.1.0	MAC OSX 10.13.4 High Sierra	libpardiso600-MACOS-X86-64.dylib, libiomp5.dylib

Other libraries can be compiled upon request. Please let us know in case that some of these libraries are not working for you. You can only download the files above if you are a registered user and agreeing to the license conditions.

Matpower Libraries

Ipopt 3.12.9 (extended version), PARDISO 6.0 (threaded version)

You need to set the numbers of threads with, for example, if you would like to use 8 cores you should use `export OMP_NUM_THREADS=8` before running ipopt.mexa64 in Matlab.

In addition, you need a PARDISO license file pardiso.lic which can be obtained here.

Architecture	Operating System	Files
Architecture x86-64, 64-bit, Matlab R2016b	Linux	ipopt.mexa64, ipopt_auxdata.m, ipopt.opt, examplehs071.m
Architecture x86-64, 64-bit, Matlab R2016b	Mac OS X 10.13.4	ipopt.mexmaci64, ipopt_auxdata.m, ipopt.opt, examplehs071.m

1-dimensional Poisson equation

- Let us assume a discrete Poisson equation in 1D Cartesian coordinates

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = f(x), \qquad x \in [0,1] \qquad u(0) = u_0 \quad \text{and} \quad u(1) = u_1,$$

- Let's discretize it, having *m* stencils (i ∈ [1, *m*]), and boundary values at i = 0 and i = m + 1.

- At i = 1, the Poisson equation then reads: $\Phi_0 - 2\Phi_1 + \Phi_2 = 4\pi G h^2 \rho_1$

The lower boundary condition Φ_0 is now shifted tothe other side of the equation:

$$-2\Phi_1 + \Phi_2 = 4\pi G h^2 \rho_1 - \Phi_0$$

The upper boundary at i = m is treated in analogy: $\Phi_{m-1} - 2\Phi_m = 4\pi G h^2 \rho_m - \Phi_{m+1}$

Hence, the Poisson equation can be casted into a matrix notation,
representing an m × m linear system of the general form

$$A\vec{\Phi} = \vec{\rho}\,.$$

Multi-dimensional Poisson equation

- In 3D Cartesian coordinates, the Poisson equation for the gravitational potential reads:

$$\Delta\Phi(x,y,z) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Phi = 4\pi G\rho(x,y,z)$$

- The discretized version of this equation (assuming a uniform spatial discretization) on an **m × n × k grid** yields the following formula:

$$\Phi_{i-1,j,k} + \Phi_{i,j-1,k} + \Phi_{i,j,k-1} - 6\Phi_{i,j,k} + \Phi_{i+1,j,k} + \Phi_{i,j+1,k} + \Phi_{i,j,k+1} = 4\pi G h^2 \rho(x,y,z)\ ,$$

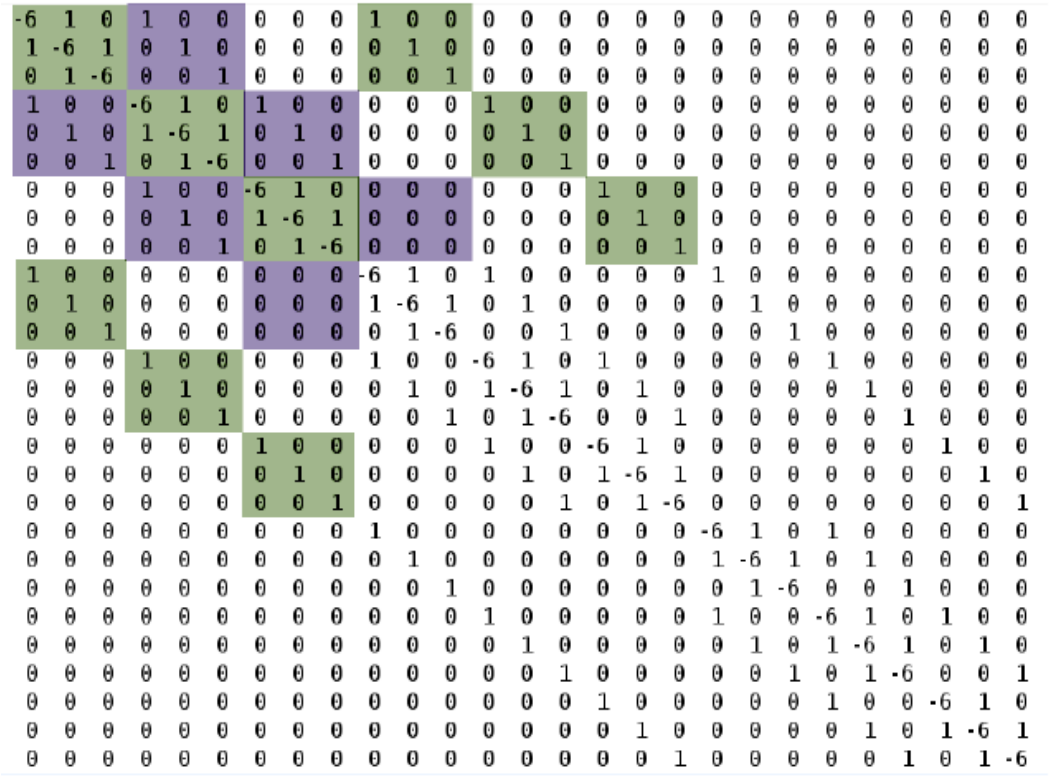
- ***h*** is the grid spacing.

- This can again be casted into a matrix notation, representing an **mnk × mnk linear system** of the general form

$$A\vec{\Phi} = \vec{\rho}\ .$$

Sparse matrix

For a 3 × 3 × 3 (m = 3, n = 3, k=3) grid with all the boundary nodes fixed (set to be zero), the matrix A of the system would look as displayed left below.
In our notation, the entries of the vectors **Φ** and **ρ** are defined as below right.



$$\vec{\Phi} = \begin{pmatrix} \Phi_{111} \\ \cdot \\ \cdot \\ \cdot \\ \Phi_{11k} \\ \Phi_{121} \\ \cdot \\ \cdot \\ \cdot \\ \Phi_{1nk} \\ \Phi_{211} \\ \cdot \\ \cdot \\ \cdot \\ \Phi_{mnk} \end{pmatrix} \quad ; \qquad \vec{\rho} = 4\pi G h^2 \begin{pmatrix} \rho_{111} \\ \cdot \\ \cdot \\ \cdot \\ \rho_{11k} \\ \rho_{121} \\ \cdot \\ \cdot \\ \cdot \\ \rho_{1nk} \\ \rho_{211} \\ \cdot \\ \cdot \\ \cdot \\ \rho_{mnk} \end{pmatrix}$$

This (and many other) PDEs can be solved by inverting the sparse matrix

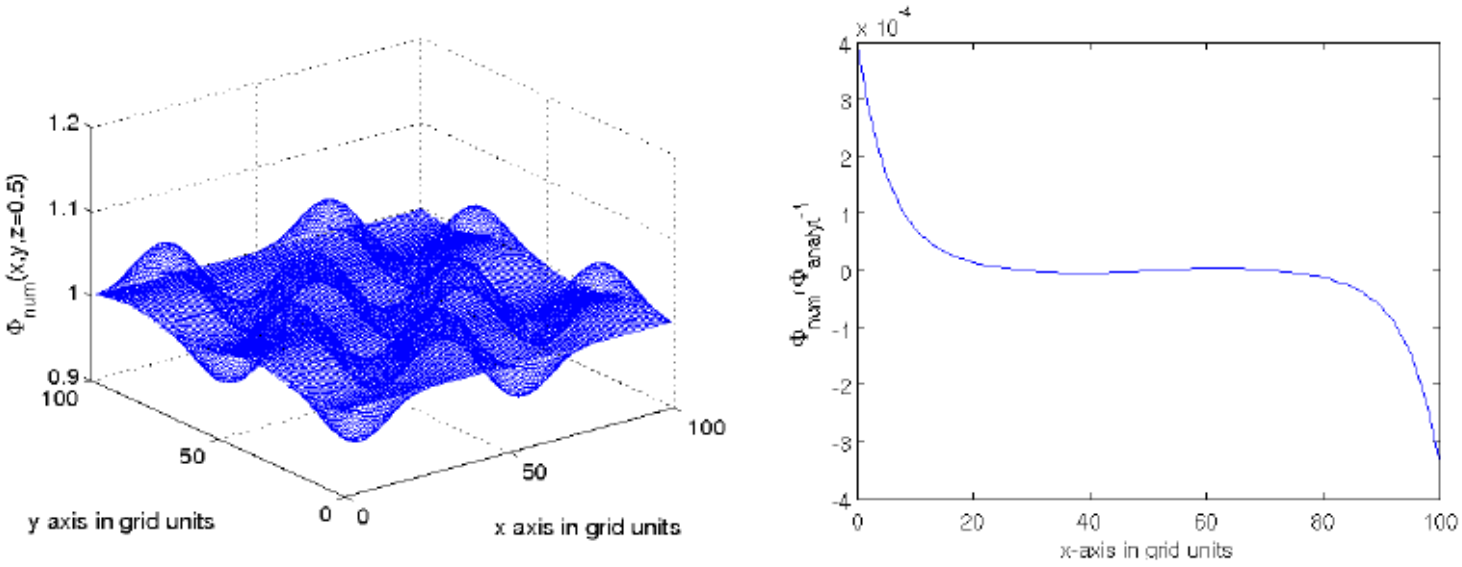
An analytical example

One exemplary analytical test: $\Delta\Phi(x,y,z) = f(x,y,z) = -48\pi^2 \sin(4\pi x)\sin(4\pi y)\sin(4\pi z)$.

Let's map the interval x, y, z ∈ 100^3 , mapped onto grid points

We impose Dirichlet boundary conditions ∂Ω = 1.

The analytical solution reads $\Phi(x,y,z) = \sin(4\pi x)\sin(4\pi y)\sin(4\pi z)$



Left panel: Numerical solution of eq. 2.85 in the $z = 0.5$ plane. **Right panel:** Relative error $\Phi_{num}(x, 0.5, 0.5)/\Phi_{analyt}(x, 0.5, 0.5) - 1$ along the x-axis.

Example

0. Prepare environment

module load Libs/GCC/5.2.0
module load Libs/netlib
module Langs/GCC/5.2.0

1. Go to

> cd YaleParallel2018/day4/code_day4/pardiso_example

2. Have a look at the code

>vi driver.f90

3. compile by typing:

> source setenv_yale.sh
> make

4. run the code

>export OMP_NUM_THREADS=1
>time ./test |tee output.txt (rather USE SLURM!!!)

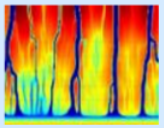
5. vary export OMP_NUM_THREADS=1,2,4,8,...

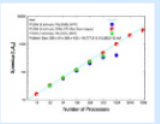
6. have a look at the profiles (profile_0000.dat)

Example: PETSc

https://www.mcs.anl.gov/petsc/

PETSc





Portable, Extensible Toolkit for Scientific Computation

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News: PETSc User Meeting, June 28-30, 2016

The current version of PETSc is 3.7; released April 25, 2016.

PETSc, **pronounced PET-see** (the S is silent), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It supports MPI, and GPUs through CUDA or OpenCL, as well as hybrid MPI-GPU parallelism.

- Scientific applications that use PETSc
- Features of the PETSc libraries (and a recent podcast)
- Linear system solvers accessible from PETSc
- Related packages that use PETSc
  - MOOSE - Multiphysics Object-Oriented Simulation Environment finite element framework, built on top of libMesh and PETSc
  - SLEPc - Scalable Library for Eigenvalue Problems
  - COOLFluiD - CFD, plasma and multi-physics simulation package
  - Fluidity - a finite element/volume fluids code
  - OpenFVM - finite volume based CFD solver
  - OOFEM - object oriented finite element library
  - libMesh - adaptive finite element library
  - FEniCS - sophisticated Python based finite element simulation package
  - Firedrake - sophisticated Python based finite element simulation package
  - DEAL.II - sophisticated C++ based finite element simulation package
  - PHAML - The Parallel Hierarchical Adaptive MultiLevel Project
  - Chaste - Cancer, Heart and Soft Tissue Environment
  - PyClaw - A massively parallel, high order accurate, hyperbolic PDE solver
  - PetIGA - A framework for high performance Isogeometric Analysis
  - **Python Bindings**
    - petsc4py from Lisandro Dalcin at CIMEC
    - Elefant from the SML group at NICTA

    Java Bindings
    - jpetsctao from Hannes Sommer (this does not appear to be functional any longer
- Packages that PETSc can optionally use

PETSc is developed as open-source, requests and contributions are welcome.

What is PETSc?

PETSc, the Portable Extendible Toolkit for Scientifc Computation, is a large powerful library, mostly concerned with linear and non-linear system of equations that arise from discretized PDEs.

PETSc can be used as a **library in the traditional** sense, where you use some **high level functionality**, such as **solving a non-linear system** of equations, in your program.

However, it **can also be used as a toolbox**, to compose your own numerical applications using low-level tools.

- Linear system solvers (sparse/dense, iterative/direct)
- Non-linear system solvers
- Tools for distributed matrices
- Support for profiling, debugging, graphical output

The basic functionality of PETSc can be extended through external packages:

- Dense linear algebra: Scalapack
- Grid partitioning software: ParMetis, Jostle, Chaco, Party
- ODE solvers: PVODE
- Eigenvalue solvers (including SVD): SLEPc
- Optimization: TAO

Why use PETSc?

- Write robust, scalable MPI codes to solve PDEs, without writing much MPI code yourself.

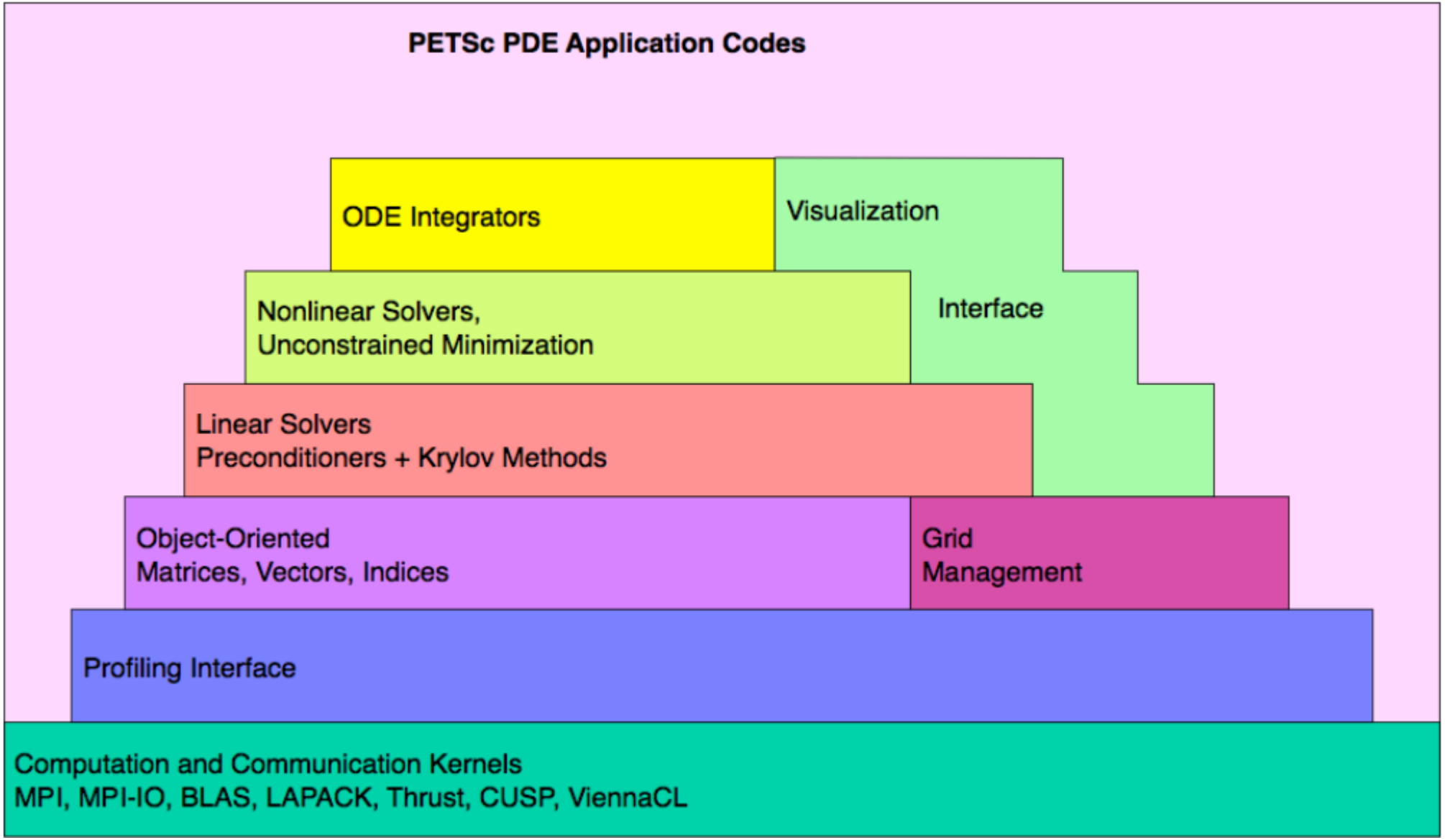
- Use a combinatorial explosion of solvers, configurable at runtime.

- Run your code essentially anywhere, from your laptop up to GRACE or other large clusters.

- Configure with a huge number of external packages (including external linear solvers).

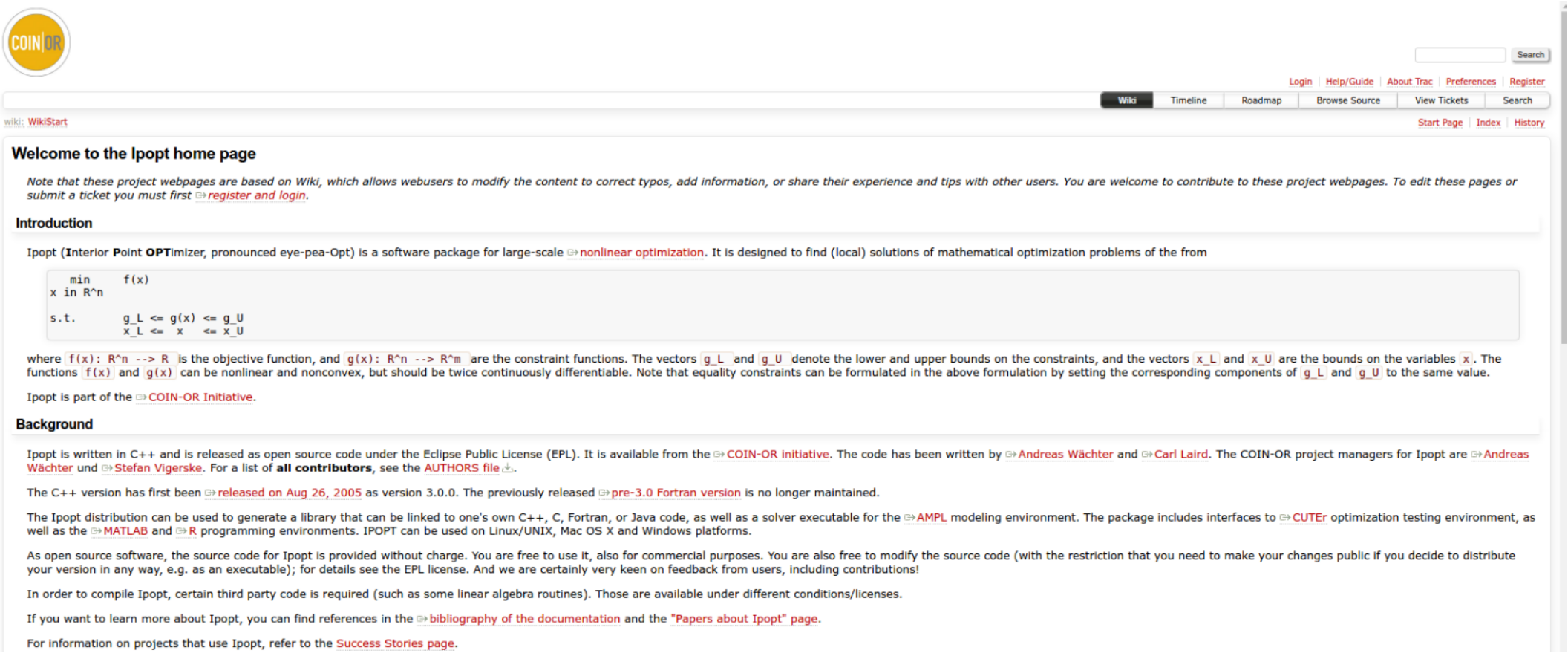
- Excellent support and community.

PETSc Components



Example: Optimization

https://projects.coin-or.org/Ipopt – we used it in one of the projects



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wiki: WikiStart

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Welcome to the Ipopt home page

Note that these project webpages are based on Wiki, which allows webusers to modify the content to correct typos, add information, or share their experience and tips with other users. You are welcome to contribute to these project webpages. To edit these pages or submit a ticket you must first register and login.

Introduction

Ipopt (**I**nterior **P**oint **OPT**imizer, pronounced eye-pea-Opt) is a software package for large-scale nonlinear optimization. It is designed to find (local) solutions of mathematical optimization problems of the from

```
   min     f(x)
x in R^n

s.t.       g_L <= g(x) <= g_U
           x_L <=  x   <= x_U
```

where `f(x): R^n --> R` is the objective function, and `g(x): R^n --> R^m` are the constraint functions. The vectors `g_L` and `g_U` denote the lower and upper bounds on the constraints, and the vectors `x_L` and `x_U` are the bounds on the variables `x`. The functions `f(x)` and `g(x)` can be nonlinear and nonconvex, but should be twice continuously differentiable. Note that equality constraints can be formulated in the above formulation by setting the corresponding components of `g_L` and `g_U` to the same value.

Ipopt is part of the COIN-OR Initiative.

Background

Ipopt is written in C++ and is released as open source code under the Eclipse Public License (EPL). It is available from the COIN-OR initiative. The code has been written by Andreas Wächter and Carl Laird. The COIN-OR project managers for Ipopt are Andreas Wächter und Stefan Vigerske. For a list of **all contributors**, see the AUTHORS file.

The C++ version has first been released on Aug 26, 2005 as version 3.0.0. The previously released pre-3.0 Fortran version is no longer maintained.

The Ipopt distribution can be used to generate a library that can be linked to one's own C++, C, Fortran, or Java code, as well as a solver executable for the AMPL modeling environment. The package includes interfaces to CUTEr optimization testing environment, as well as the MATLAB and R programming environments. IPOPT can be used on Linux/UNIX, Mac OS X and Windows platforms.

As open source software, the source code for Ipopt is provided without charge. You are free to use it, also for commercial purposes. You are also free to modify the source code (with the restriction that you need to make your changes public if you decide to distribute your version in any way, e.g. as an executable); for details see the EPL license. And we are certainly very keen on feedback from users, including contributions!

In order to compile Ipopt, certain third party code is required (such as some linear algebra routines). Those are available under different conditions/licenses.

If you want to learn more about Ipopt, you can find references in the bibliography of the documentation and the "Papers about Ipopt" page.

For information on projects that use Ipopt, refer to the Success Stories page.

Emerging hardware

GPU: NVIDIA Tesla K20c

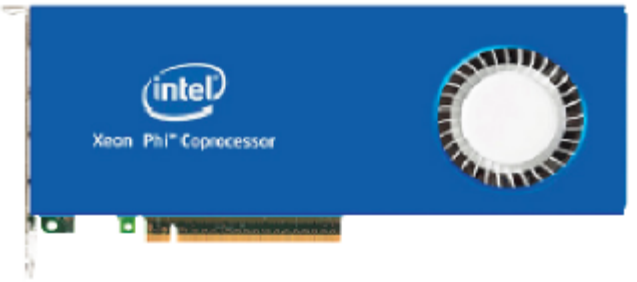
Kepler GK110, 28 nm

13 mp × 192 cores @ 0.71 GHz

5 GB GDDR5 @ 2.6 GHz

225W

→ **Devices can have *O(Teraflops)***



MIC: Intel Xeon Phi 3120A

Knights Corner (KNC), 22 nm

57 cores @ 1.1 GHz

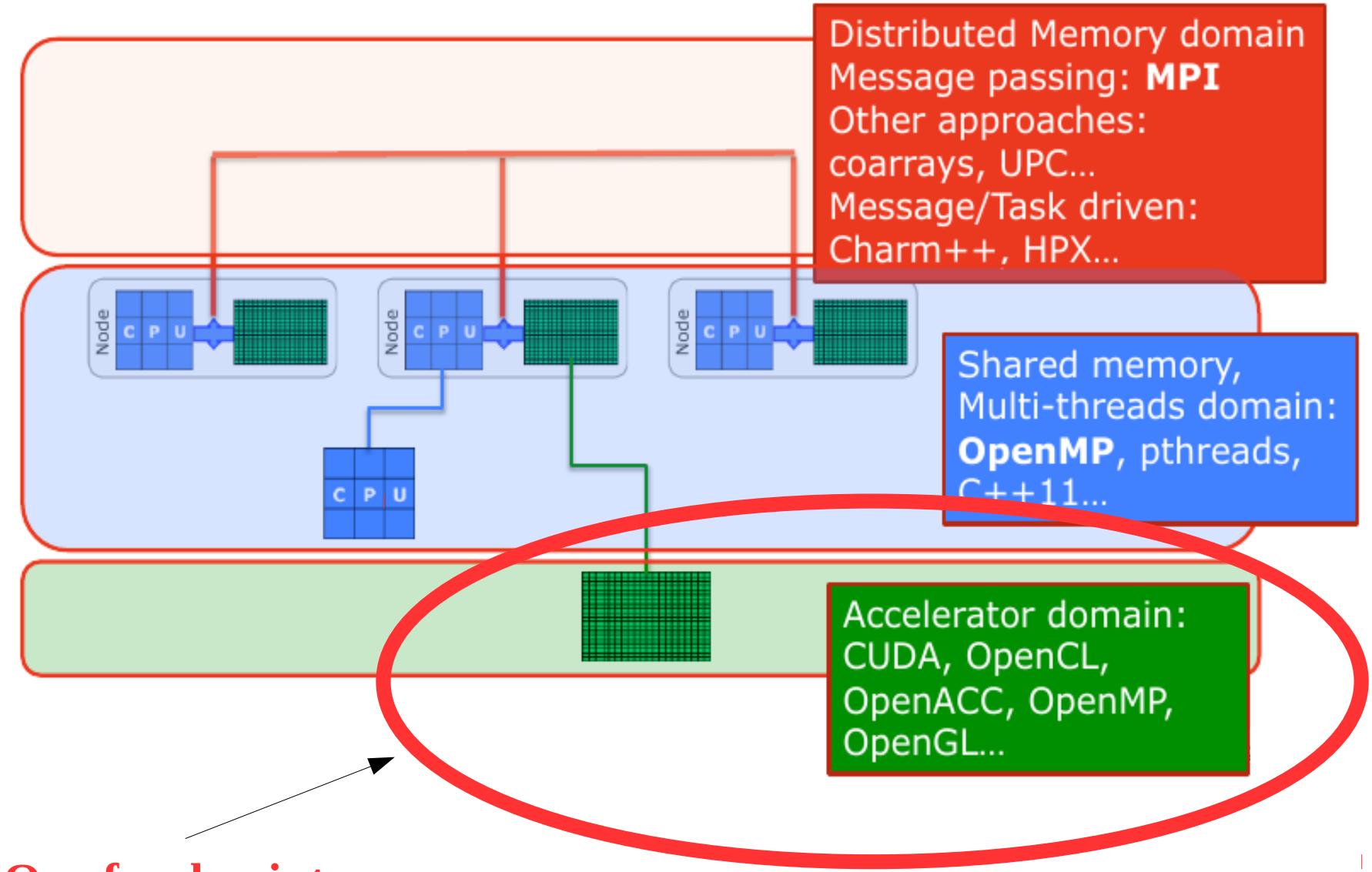
6GB GDDR5 @ 1.1 GHz

300W

up to 4 threads per core

512-bit vectorization (AVX-512)

Overall picture of programming models



(Slide from C. Gheller)

Why do we Need Co-processors/or "Accelerators" on HPC?

- In the past, computers got faster by increasing the **clock frequency** of the core, but this has now reached its limit mainly due to **power requirements** and heat dissipation restrictions (unmanageable problem).

- **Today, processor cores are not getting any faster, but instead the number of cores per chip increases.**

- **On HPC, we need a chip that can provide higher computing performance at lower energy.**

General Purpose GPU

- Graphics Processing Unit (GPU):
  → Hardware designed for output to display.

- **General Purpose computing on GPUs (GPGPU)**:

  → Use GPUs for **non-graphics tasks,** e.g. physics simulation, signal processing, computational geometry, computer vision, database management, computational biology, computational finance

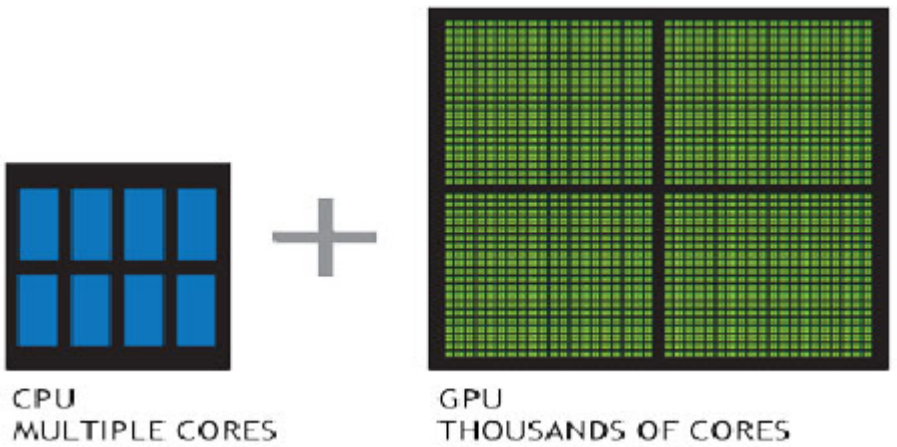
- GPUs evolved into a very flexible and powerful processor:
  → It’s programmable using high-level languages

Solution

- The actual solution is a heterogeneous system containing both CPUs and “accelerators”, plus other forms of parallelism such as vector instruction support.

- Widely accepted that heterogeneous systems with accelerators deliver the highest performance and energy efficient computing in HPC.

- Today – the accelerated computing is revolutionising HPC.



Top 500 – June 2018 (het. systems)

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,282,544	122,300.0	187,659.3	8,806
2	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
3	**Sierra** - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/NNSA/LLNL United States	1,572,480	71,610.0	119,193.6	
4	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 , NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482
5	**AI Bridging Cloud Infrastructure (ABCI)** - PRIMERGY CX2550 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR , Fujitsu National Institute of Advanced Industrial Science and Technology (AIST) Japan	391,680	19,880.0	32,576.6	1,649
6	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray Inc. Swiss National Supercomputing Centre (CSCS) Switzerland	361,760	19,590.0	25,326.3	2,272
7	**Titan** - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x , Cray Inc. DOE/SC/Oak Ridge National Laboratory United States	560,640	17,590.0	27,112.5	8,209
8	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom , IBM DOE/NNSA/LLNL United States	1,572,864	17,173.2	20,132.7	7,890
9	**Trinity** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray Inc. DOE/NNSA/LANL/SNL United States	979,968	14,137.3	43,902.6	3,844
10	**Cori** - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect , Cray Inc. DOE/SC/LBNL/NERSC United States	622,336	14,014.7	27,880.7	3,939

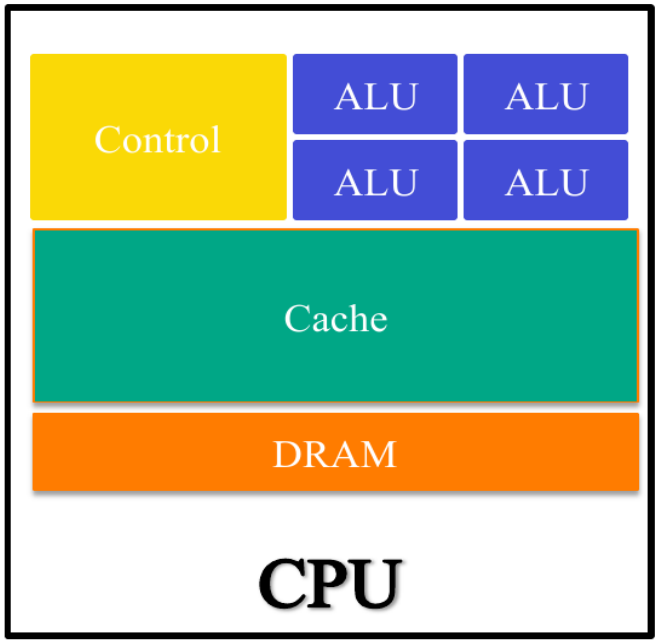
CPU vs. GPU

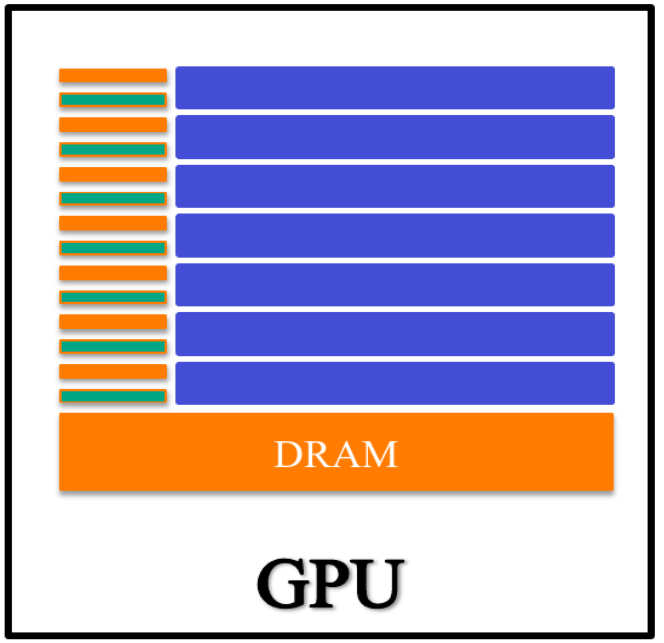
- Specialized for compute-intensive, highly-parallel computation, i.e. graphic output.

- Evolution pushed by gaming industry.

- CPU: large die area for control and caches.

- GPU: large die area for data processing.





Programming GPUs

- CUDA: Nvidia proprietary API, works only on Nvidia GPUs.

- OpenCL: open standard for heterogeneous computing.

- OpenACC: open standard based on compiler directives.

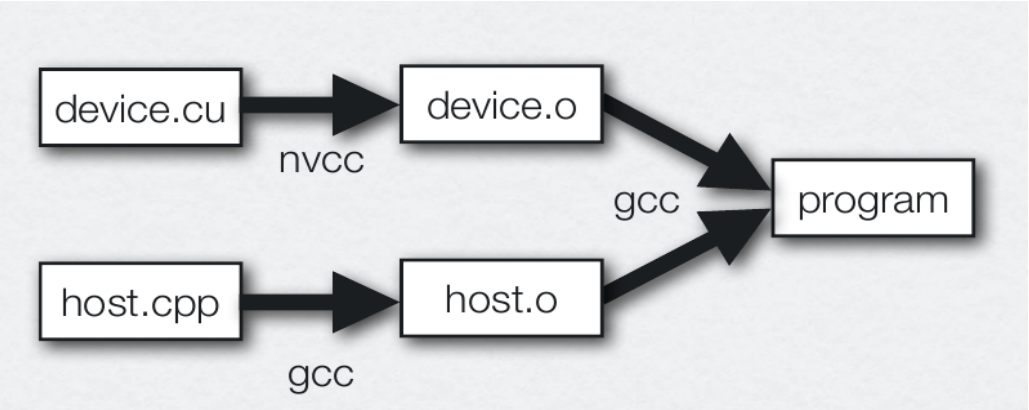
Nvidia CUDA

- Compute Unified Device Architecture (CUDA)

- C extension to write GPU code, support for C++

- Only supported by Nvidia GPUs

- Code compilation (nvcc) and linking:



device.cu

```
__global__ void kernel()
{
    // do something
}
```

host.cpp

```
int main()
{
}
```

OpenACC

- Programming with CUDA can be more difficult than writing SPMD applications.

→ **OpenACC (Open Accelerators)**

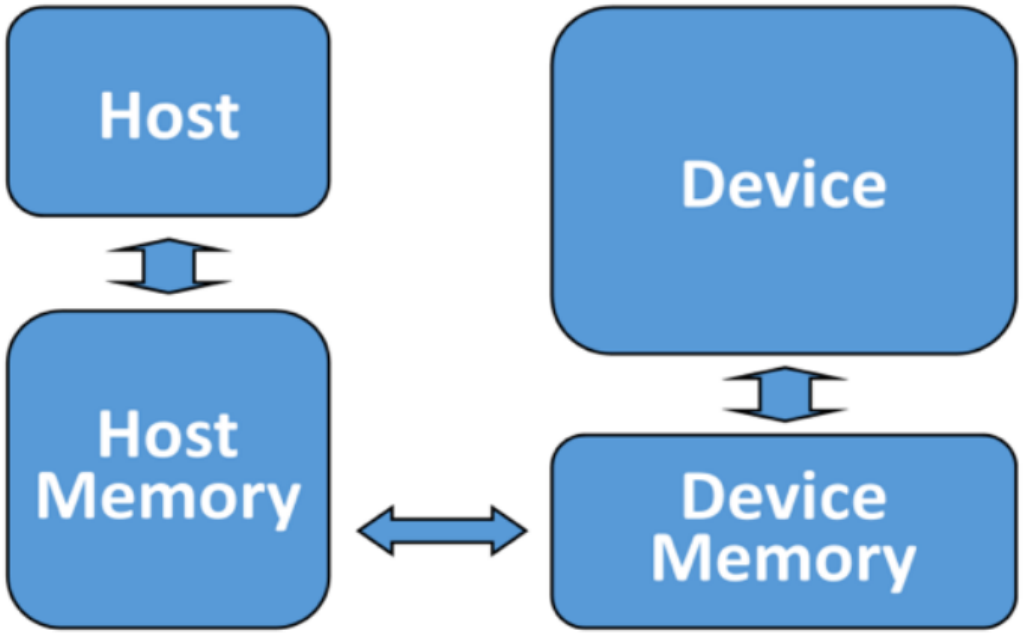
- Developed by Cray, CAPS, Nvidia, and PGI.
- Most recent specification: 2.5 (November 2015).
- Similar to OpenMP.
- High-level of abstraction.
- OpenACC members are also part of the OpenMP language committee.
- Compiler support from Cray, PGI, and CAPS.
- Experimental support for OpenACC in GCC/5.1.

OpenACC

- The **OpenACC API is a set of compiler directives** for offloading work to accelerators.

- For many systems, there will is a CPU host and GPU accelerator.

- **OpenACC will handle any accelerator memory management and the transfer of data**.



OpenACC Abstract Accelerator

Directives

- Like OpenMP, OpenACC is primarily programmed using directives.
- Lower-level programming models like CUDA perform better for certain optimizations (i.e. abstraction penalty).

C/C++

#pragma acc directive-name [clause-list] new-line

Scope is the following block of code

Fortran

!$acc directive-name [clause-list] new-line

Scope is until **!$acc end** directive name

```
 9 #pragma acc parallel loop
10   for (i=0;i<N;i++) {
11     y[i] = 0.0;
12     x[i] = (double) (i+1);
13   }
14
```

Intel Xeon Phi Products

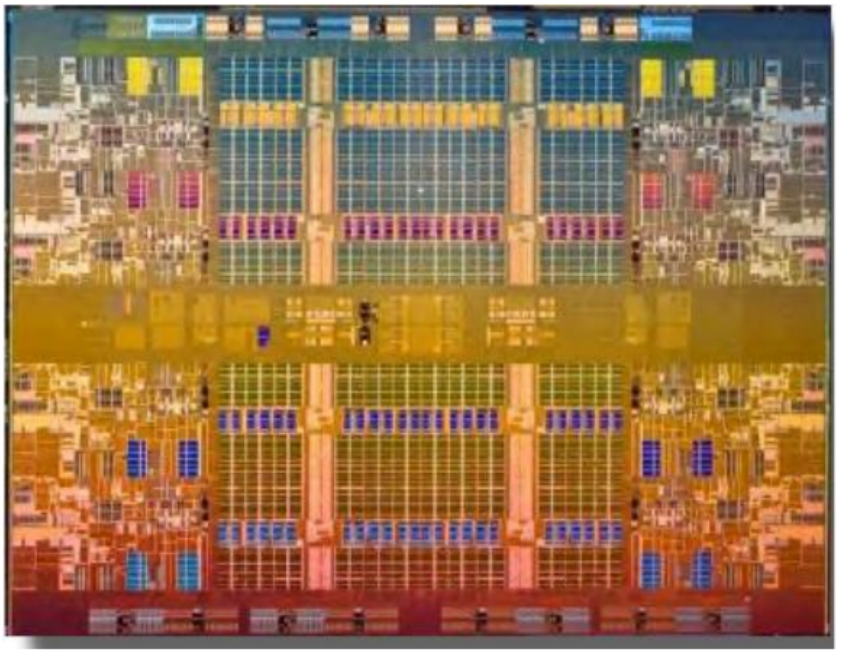
- The first product was released in 2012 named **Knights Corner (KNC)** which is the first architecture supporting **512 bit vectors**.

- The 2nd generation released last week named **Knights Landing (KNL)** also support 512bit vectors with a new instruction set called Intel Advanced Vector Instructions 512 (Intel AVX-512).

- KNL has a peak performance of **6 TFLOP/s in single precision** ~ 3 times what KNC had, due to 2 **vector processing units (VPUs)** per core, doubled compared to the KNC.
  → Each VPU operates independently on 512-bit vector registers, which can hold 16 single precision or 8 double precession floating-point numbers.

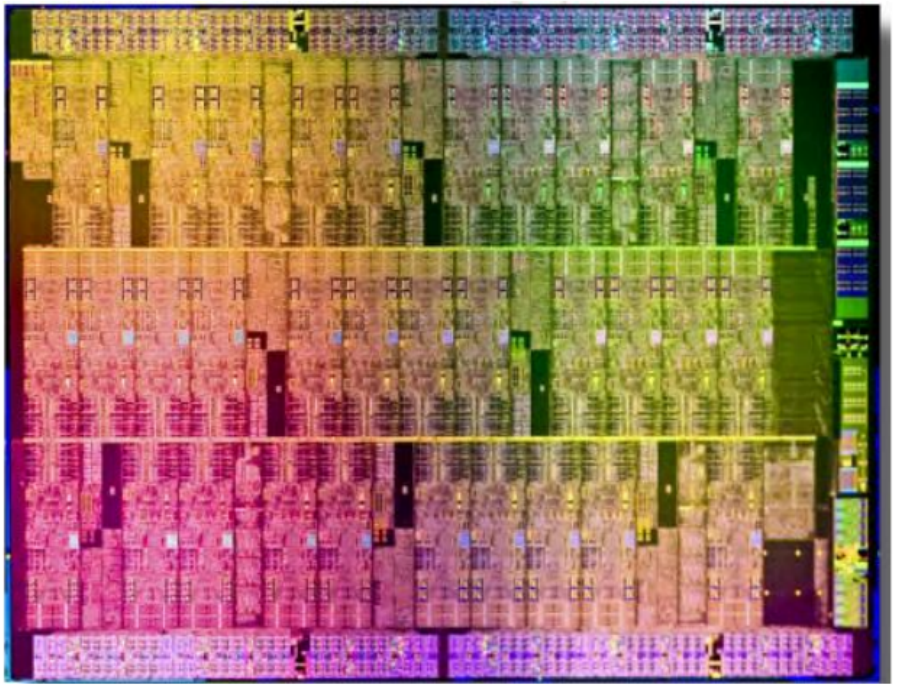
Multi-core vs. Many-core

Parallel Programming and Optimization with Intel Xeon Phi Coprocessors, Colfax 2013
http://www.colfaxintl.com/nd/xeonphi/book.aspx



Multi-core Intel Xeon processor

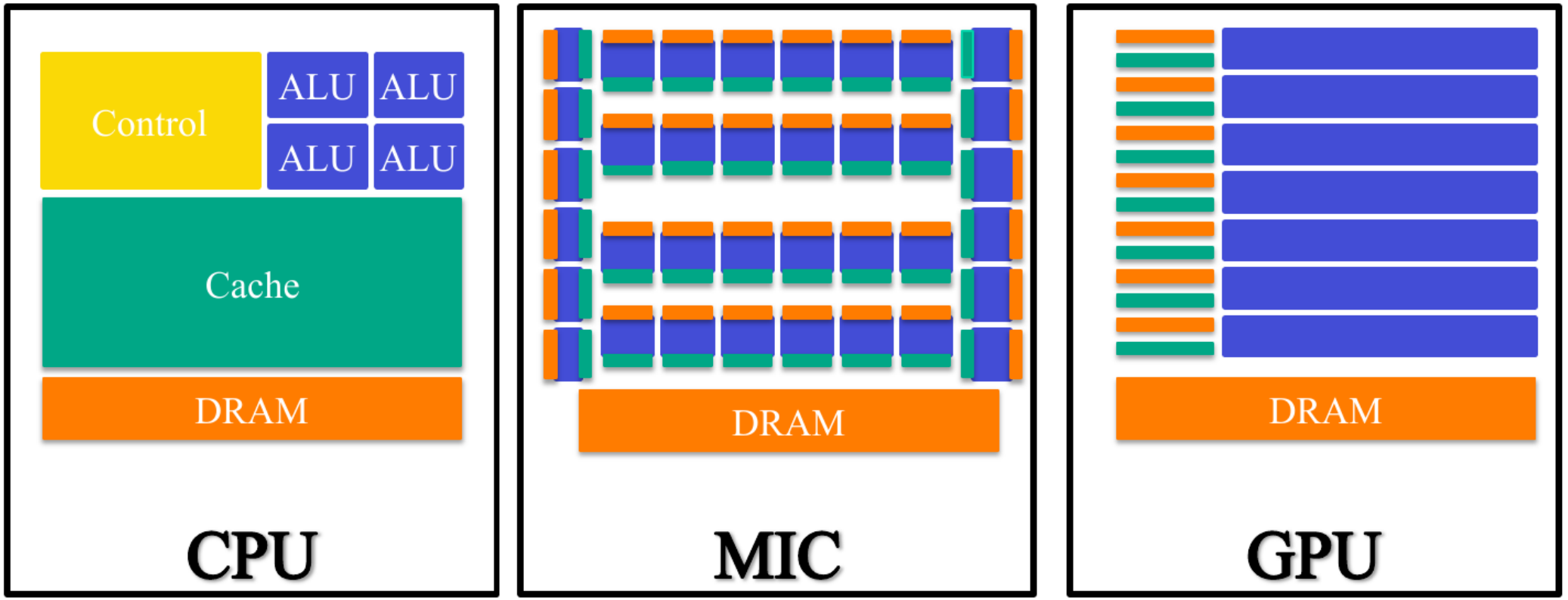
- ~ 16 physical cores ~ 3 GHz
- e.g Intel Sandy-Bridge 32 nm
- (AVX) 256-bit vector registers



Many-core Intel Xeon Phi coprocessor

- ~ 61 cores (244) ~ 1 GHz
- 22 nm
- 512-bit vector registers

Architecture comparison



General-purpose architecture

Power-efficient

Multiprocessor X86 design architecture

Massively data parallel

Advantages of MIC

- Retains programmability and flexibility of standard x86 architecture.

- No need to learn a new complicated language like CUDA or OpenCL.

- Offers possibilities we miss on GPUs: Login onto the system, watching and controlling processes via top, kill etc. like on a Linux host.

- **Allows many different parallel programming models like OpenMP, MPI, and Intel Threading Building Blocks (TBB)**.

- Offers standard math-libraries like Intel MKL.

- **Supports whole Intel tool chain**, e.g. Intel C/C++ and Fortran Compiler, Debugger & Intel VTune Amplifier.

High throughput computing/Cloud

Definition of cloud computing

Cloud computing enables users to consume a compute resource, such as a virtual machine (VMs), storage or an application, as a utility – **just like electricity** – rather than having to build and maintain computing infrastructures in house.

Cloud computing boosts several attractive benefits for end users. Three of the main benefits of cloud computing are:

→ Self-service provisioning: End users can spin up compute resources for almost any type of **workload on demand**. This eliminates the traditional need for IT administrators to provision and manage compute resources.

→ Elasticity: Users can scale up as computing needs increase and scale down again as demands decrease. This eliminates the need for massive investments in local infrastructure which may or may not remain active.

→ Pay per use: Compute resources are measured at a granular level, allowing users to pay only for the resources and workloads they use.

Examples: Amazon's EC2 compute service; Amazon S3 storage service; Apple's MobileMe (storage, file sharing, etc.); Flickr, Netflix, YouTube; etc.

High throughput computing (HTC)

- **High-throughput computing (HTC)** is a computer science term to describe the use of many computing resources over long periods of time to accomplish a computational task.

- Using distributed computing (potentially grid computing) to enable lots of jobs to be scheduled to available resources to complete as fast as possible.

- The term was popularized e.g. by Condor project (U Wisconsin).

- Examples: Condor, World Community Grid, LHC project, Open Science Grid, etc.

- Goal: to integrate multiple computing systems to enable large numbers of tasks to be schedule and completed as rapidly as possible. Resources: can be centrally managed servers (clusters, clouds) and/or distributed PCs.

Example – HTCondor

https://research.cs.wisc.edu/htcondor/
http://chtc.cs.wisc.edu/

Grid Computing Definition*

*https://en.wikipedia.org/wiki/Grid_computing

Grid computing is the most distributed form of parallel computing.

It makes use of computers communicating over the Internet to work on a given problem.

Because of the low bandwidth and extremely **high latency** available on the Internet, distributed computing typically deals only with **embarrassingly parallel** problems.

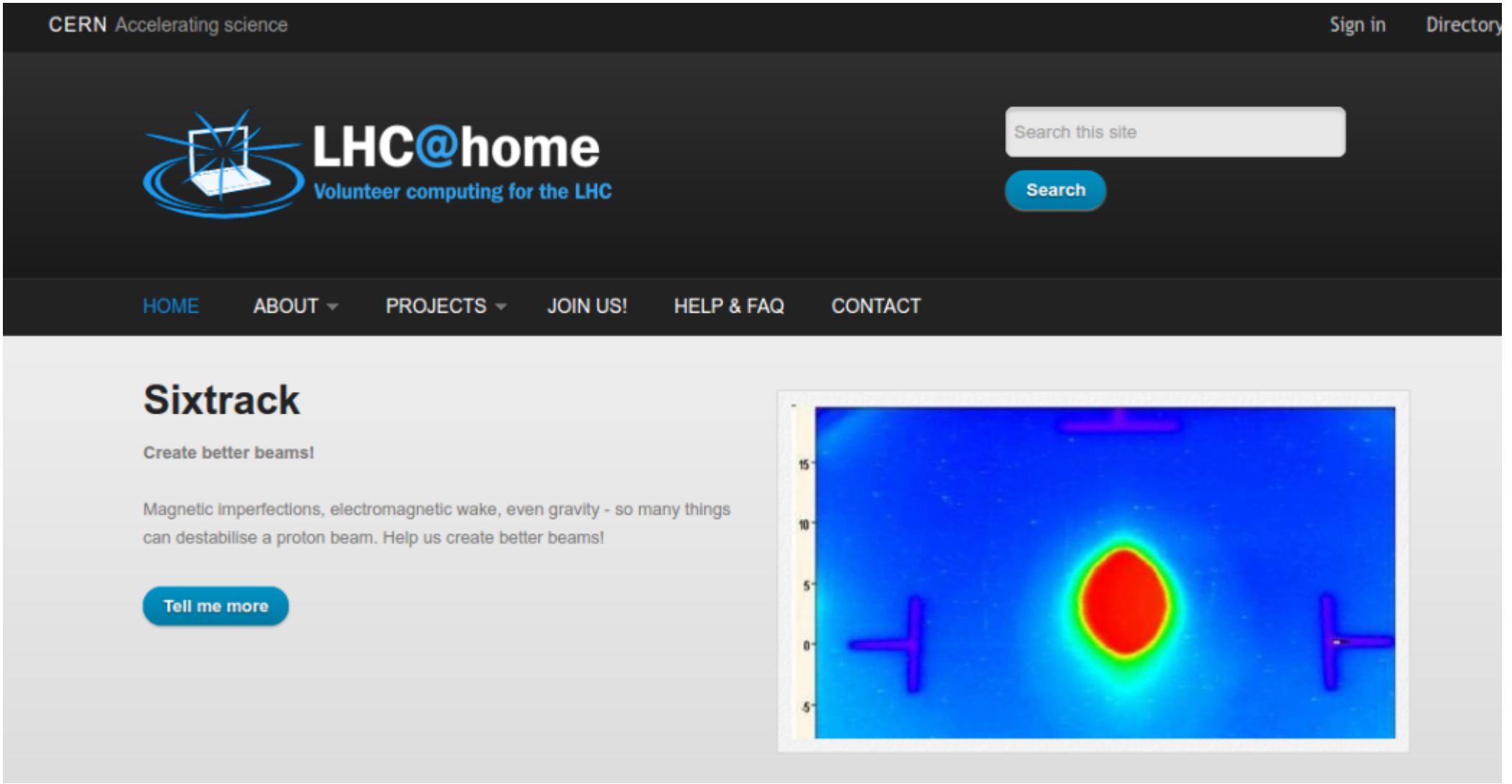
Many distributed computing applications have been created, of which **SETI@home, LHC@home and Folding@home** are the best-known examples.

Most grid computing applications use middle-ware, software that sits between the operating system and the application to **manage network resources** and standardize the software interface.

Often, distributed computing software makes use of "spare cycles", performing computations at times when a computer is idling.

Example – LHC@home

http://lhcathome.web.cern.ch/



The value of HTC

- Majority of computational science is performed on workstations/PCs
  - → HPC systems not needed for all tasks.
  - → Many tasks need to be repeated a lot.

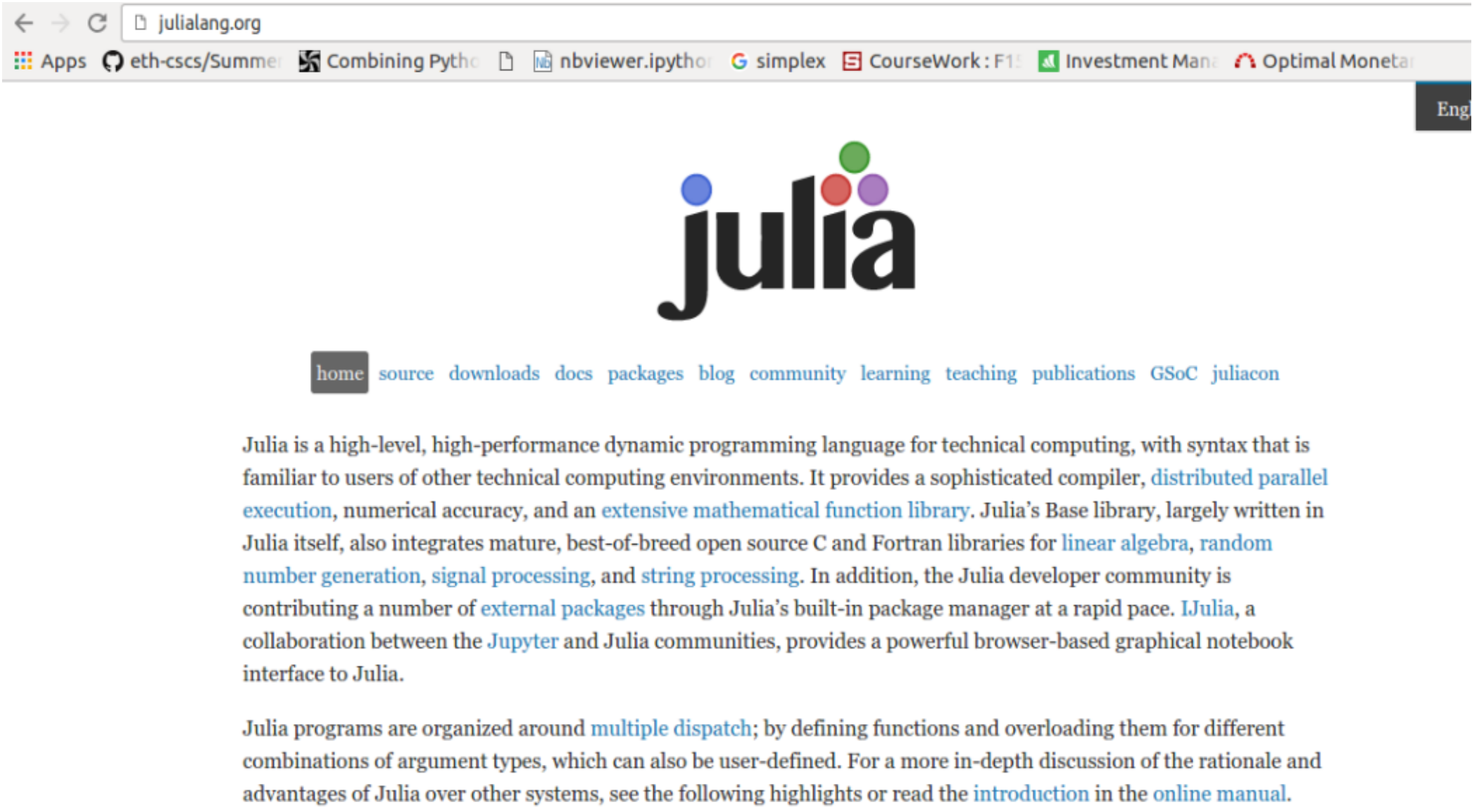
- Running simulations to explore a parameter space
  - → Running simulations on different data sets.
  - → Analyzing experimental results that ongoing/repeated.

- HTC tools enable this, sometimes from the desktop (e.g. Condor)

- Think of Big Data analytics... (http://lhcathome.web.cern.ch/)

Trending topics

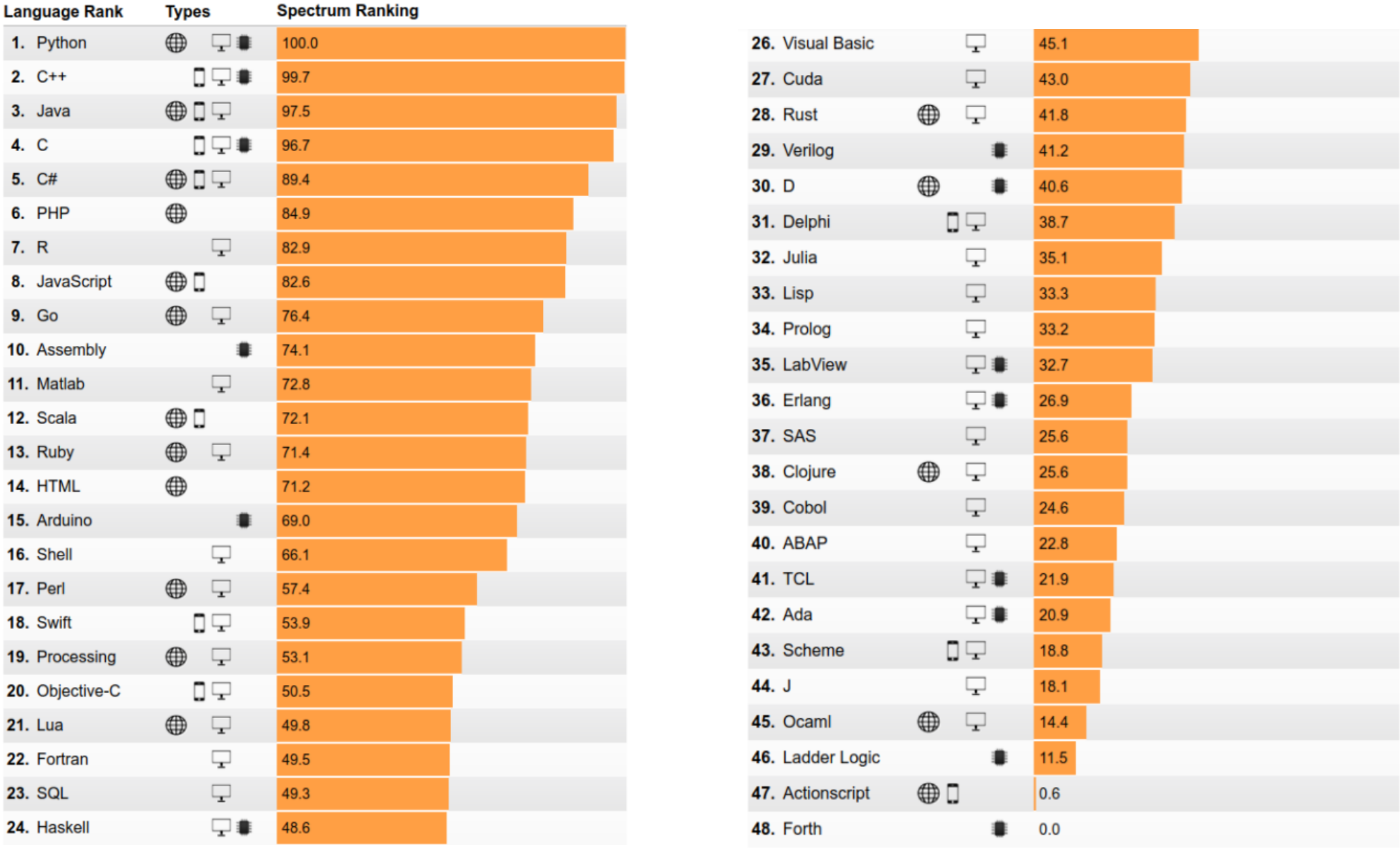
http://julialang.org/learning/
https://en.wikipedia.org/wiki/Julia_(programming_language)



Trending topics

IEEE – The Top Programming Languages 2018

*https://spectrum.ieee.org/static/interactive-the-top-programming-languages-2018



Language Rank	Types	Spectrum Ranking
1. Python	web, desktop, embedded	100.0
2. C++	mobile, desktop, embedded	99.7
3. Java	web, mobile, desktop	97.5
4. C	mobile, desktop, embedded	96.7
5. C#	web, mobile, desktop	89.4
6. PHP	web	84.9
7. R	desktop	82.9
8. JavaScript	web, mobile	82.6
9. Go	web, desktop	76.4
10. Assembly	embedded	74.1
11. Matlab	desktop	72.8
12. Scala	web, mobile	72.1
13. Ruby	web, desktop	71.4
14. HTML	web	71.2
15. Arduino	embedded	69.0
16. Shell	desktop	66.1
17. Perl	web, desktop	57.4
18. Swift	mobile, desktop	53.9
19. Processing	web, desktop	53.1
20. Objective-C	mobile, desktop	50.5
21. Lua	web, desktop	49.8
22. Fortran	desktop	49.5
23. SQL	desktop	49.3
24. Haskell	desktop, embedded	48.6
26. Visual Basic	desktop	45.1
27. Cuda	desktop	43.0
28. Rust	web, desktop	41.8
29. Verilog	embedded	41.2
30. D	web, embedded	40.6
31. Delphi	mobile, desktop	38.7
32. Julia	desktop	35.1
33. Lisp	desktop	33.3
34. Prolog	desktop	33.2
35. LabView	desktop, embedded	32.7
36. Erlang	desktop, embedded	26.9
37. SAS	desktop	25.6
38. Clojure	web, desktop	25.6
39. Cobol	desktop	24.6
40. ABAP	desktop	22.8
41. TCL	desktop, embedded	21.9
42. Ada	desktop, embedded	20.9
43. Scheme	mobile, desktop	18.8
44. J	desktop	18.1
45. Ocaml	web, desktop	14.4
46. Ladder Logic	embedded	11.5
47. Actionscript	web, mobile	0.6
48. Forth	embedded	0.0

Apache Hadoop

Apache Hadoop (2)

https://en.wikipedia.org/wiki/Apache_Hadoop
http://hadoop.apache.org/
https://www.tutorialspoint.com/hadoop/hadoop_introduction.htm

- Apache Hadoop is an open-source software framework for distributed storage and distributed processing of very large data sets on computer clusters built from commodity hardware.

- All the modules in Hadoop are designed with a fundamental assumption that hardware failures are common and should be automatically handled by the framework.

- The core of Apache Hadoop consists of a storage part, known as **Hadoop Distributed File System (HDFS)**, and a processing part called **MapReduce**.

- Hadoop splits files into large blocks and distributes them across nodes in a cluster.

- To process data, Hadoop transfers packaged code for nodes to process in parallel based on the data that needs to be processed.

- This approach takes advantage of data locality – nodes manipulating the data they have access to – to allow the dataset to be processed faster and more efficiently than it would be in a more conventional supercomputer architecture that relies on a parallel file system where computation and data are distributed via high-speed networking.

Quantum Computing – industry explosion

The New York Times

Microsoft Spends Big to Build a Computer Out of Science Fiction

By JOHN MARKOFF NOV. 20, 2016

THE WALL STREET JOURNAL.

Google Backs Second Quantum Computing Effort

By DON CLARK
Sep 2, 2014 9:37 pm ET

Companies building quantum computing hardware:

Microsoft IBM Google

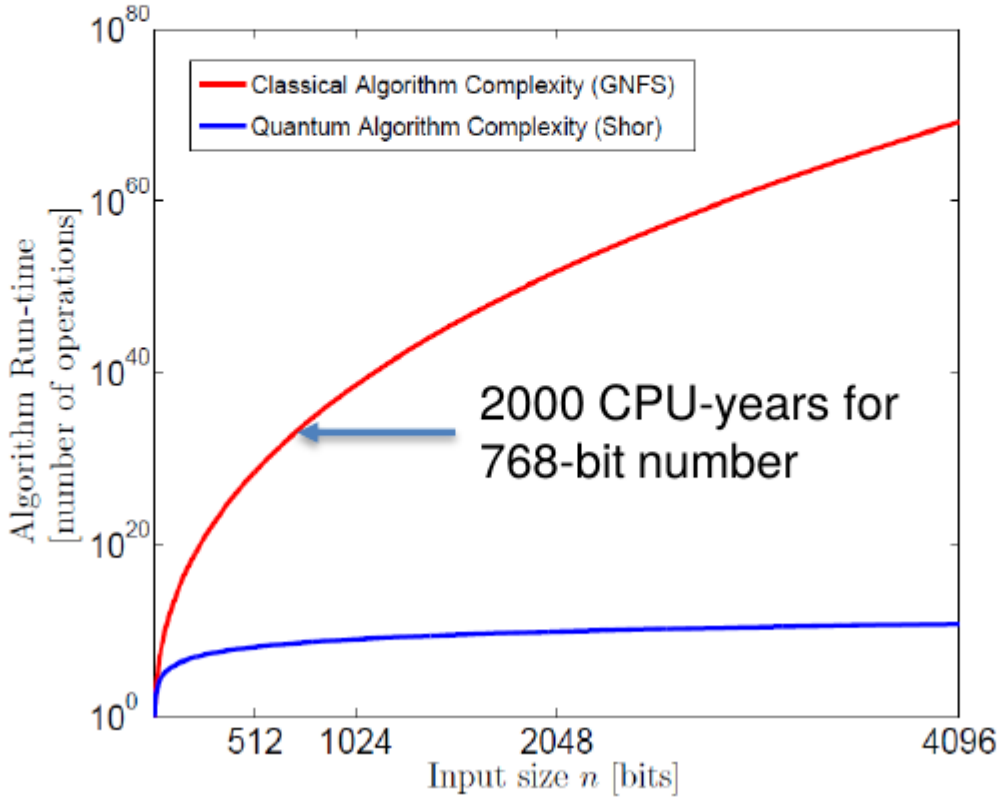
rigetti HRL LABORATORIES ION D:wave

3

Slide: courtesy of P. McMahon

The promise of quantum computing

***Vastly* faster computation for some very specific problems.**



What is a quantum computer?

A computer that fundamentally takes advantage of the laws of quantum mechanics to solve problems.

(Quantum mechanics is the theory of how physical systems behave, and is typically relevant only when the system is very small.)

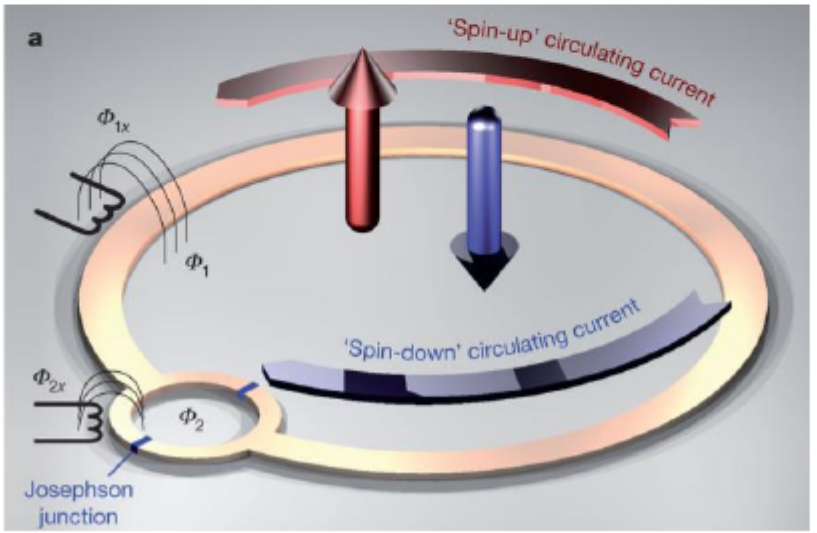


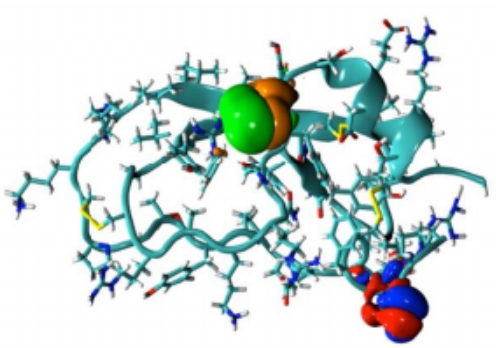
Image credit: M.W. Johnson, et al. *Nature* **473**, 194 (2011)

What is a quantum computer good for?

There are two major applications of quantum computing that the community is very convinced about. There are several others that are more speculative.

Quantum Chemistry

Calculation of chemical properties from first principles.



17% of Oak Ridge National Lab **supercomputer time** is spent on quantum chemistry (source: Juerg Hutter, 2011)

Prime Factoring

Breaking a product of two prime numbers into its prime factors (main use: breaking modern public-key cryptography systems)

15 = 3 x 5

642469 = 601 x 1069

Substantial resources are required for classical algorithms: **2000 CPU-years** for **768-bit** number

Slide: courtesy of P. McMahon

Moving forward

- Quantum computer hardware development now has strong industrial backing (Google, Microsoft, IBM, etc.)
- Google is expected to demonstrate "quantum supremacy" for the first time within the next year using a 49-qubit machine
- Google is aiming to reach 1 million physical qubits by 2027
- IBM will release a 17-qubit machine this year (and has 5-qubit machine available already)
- There are two well-established areas in which QC will give an advantage (chemistry and cryptography breaking)
- Discovering other areas is an active area of research

Wrap-up (1)

Lecture 1

1. Introduction to parallel and high-performance computing.

2. Introduction to a (discrete state) dynamic programming code in C++.

Lecture 2

1. Introduction to OpenMP (shared-memory parallelization).

2. A shared memory parallel dynamic programming code.

Wrap-up (2)

Lecture 3

1. Introduction to MPI (distributed-memory parallelization).
2. A distributed memory parallel dynamic programming code.

Lecture 4:

1. Hybrid parallelism – OpenMP & MPI.
2. A hybrid parallel dynamic programming code.
3. Advanced topics.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CALM
AND
ACCEPT THE FACT
THAT IT'S OVER
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